

# Effective relational dynamics of the closed FRW model universe minimally coupled to a massive scalar field

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## Abstract

We apply the effective approach to evaluating semiclassical relational dynamics to the closed Friedman–Robertson–Walker cosmological model filled with a minimally coupled massive scalar field. This model is interesting for studying relational dynamics in a more general setting because (i) it features a non-trivial coupling of the relational clock to the evolving degrees of freedom, (ii) no temporally global clock variable exists, and, (iii) it is non-integrable which is typical for generic dynamical systems. The effective approach is especially well-gearred for addressing the concept of relational evolution in this context since it enables one to switch between different clocks and yields a consistent (temporally) local time evolution with transient observables so long as semiclassicality holds. We provide evidence that relational evolution in this model universe, while possible for sufficiently semiclassical states, generically breaks down in the region of maximal expansion. This is rooted in a defocussing of classical trajectories which leads to a rapid spreading of states that are initially sharply peaked and to a mixing of internal time directions in this region. These results are qualitatively compared to previous work on this model, revisiting conceptual issues that have been raised earlier in the literature.

## 1 Introduction

“How can a unitary evolution in a ‘classical’ time emerge from the full quantum theory?” This question is one of the central conundrums in quantum gravity and cosmology and constitutes one of the many facets of the problem of time [1, 2, 3, 4, 5]. It is rooted in the absence of a time coordinate in the quantum theory and in the necessity to, instead, employ dynamical degrees

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of freedom to keep track of (an internal) time [6]. Such relational clock variables, however, are not perfect monotonic and classical clocks whose increment coincides with the increment of some observer’s proper time. Rather, they are genuine quantum degrees of freedom subject to quantum fluctuations and even classically will generically not always run forward, leading to what is known as the *global problem of time* [1, 2, 3, 4]. Imperfect relational clocks generically couple to other degrees of freedom of the system which causes back-reaction and complicates a good resolution of the evolution of the remaining degrees of freedom in such a clock [7, 8, 9]. In particular, a good resolution of unitary relational quantum evolution requires an approximate division between the degrees of freedom to be measured and the clock. This division is state-dependent and may, in fact, become impossible in highly quantum states [3, 4, 7, 8, 9]. The challenge of recovering a unitary evolution in a ‘classical’ internal time is thus a highly non-trivial one even in the semiclassical regime.

Extracting dynamical information from finite dimensional systems as in (loop) quantum cosmology is generally achieved by deparametrizations in specific matter degrees of freedom, such as dust or free scalar fields (or model specific geometrical degrees of freedom [10]), which assume the role of internal clocks and a lot of progress has been made in this direction [11, 12]. However, the standard free scalar field [12], as well as the recently discussed dust fields [13] decouple from the other degrees of freedom, yield a ‘time-independent’ Hamiltonian and correspond to the ‘ideal clock limit’ of [7]. These matter clocks are therefore rather special in nature.

Furthermore, the issue of non-integrability, despite being the generic case in dynamical systems [14] and having severe implications for relational evolution, has largely been overlooked in the literature on relational dynamics. Specifically, in such a situation the only global constant of motion (i.e. Dirac observable for constrained systems) is the Hamiltonian (constraint) [14]. Nevertheless, (relational) observables can still exist implicitly and locally and thus relational evolution is at least *locally* (in ‘time’) meaningful.

Advancing to more generic situations in quantum cosmology quickly leads to technical challenges such as, e.g., constructing a positive-definite inner product on the space of solutions to the quantum constraints, known as the *Hilbert space problem* [1, 2]. In order to sidestep the *Hilbert space problem* and extract qualitative and generic features from systems otherwise too intricate to be solved exactly, effective techniques have been developed [11, 15, 16, 17]. Based on these techniques an *effective approach to the problem of time* has been recently introduced [3, 4] (see also [18] for a brief summary) which allows to evaluate the relational quantum dynamics of systems featuring the *global time problem* in the semiclassical regime. This effective approach seems especially well-suited for analyzing semiclassical dynamics of non-integrable systems, for two of its main achievements are, firstly, to make sense of (temporally) local time evolution with (temporally) local relational observables and, secondly, to cope with imperfect clocks by allowing one to explicitly switch back and forth between different internal times, thereby avoiding clock pathologies. In this manner—and in analogy to local coordinates on a manifold—one is enabled to cover semiclassical evolution trajectories by patches of local relational times. In [4] this effective approach was applied to two simple toy models with decoupled clocks.

It is the goal of the present article to take a step away from deparametrizations with ‘ideal clocks’, making a first step towards the generic situation by considering (more realistically) coupled clock degrees of freedom in a non-integrable cosmological model. Concretely, although observationally a flat universe seems to be favored [19], we shall investigate the closed Friedman–Robertson–Walker (FRW) model filled with a minimally coupled massive scalar field in order to specifically address the issue of relational evolution. This model universe has been studied extensively in the literature [20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31], in particular, because it constitutes a simple cosmology which ‘generically’ produces inflation.<sup>1</sup> While the classical

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<sup>1</sup>In fact, it would be interesting to extend the nice results [32], obtained in the context of loop quantum cosmology and concerning the (essentially certain) *a priori* probability of inflation for the flat FRW model with

dynamics of this system are understood in detail [22, 25, 26, 28], its complete and consistent quantization is still pending in any approach to quantum cosmology. The troubles in constructing a complete quantization are rooted in the classical non-integrability and the absence of a (temporally) global internal clock, which leads to non-unitarity and thus far impeded discussion of relational evolution. In the main body of this article we shall explain some of the quantum troubles and—at least in the semiclassical regime—make some headway as regards relational evolution in this model universe by means of the effective approach. Whereas the resolution of the classically singular region through a quantum bounce in effective loop quantum cosmology was studied in [31],<sup>2</sup> we will rather focus on the region of maximal expansion which features a chaotic scattering and is thus especially challenging for relational dynamics.

Much attention will be devoted to conceptual issues raised in the earlier literature as regards the initial value problem and the semiclassical limit [5, 24, 30]. The primary result of the present work is strong evidence, that quantum relational evolution in this model, while possible for sufficiently semiclassical states, generically breaks down in the region of maximal expansion; non-integrability leads to a defocussing of nearby classical trajectories and thereby to a breakdown of semiclassicality. In addition, the chaotic behavior of the model can lead to a complicated structure of phase space orbits on all scales, making it fundamentally impossible to construct semiclassical states peaked around a large class of classical orbits. These results shed a first light on (the breakdown of) relational quantum evolution in generic situations and highlight the nontrivial nature of the question posed in the beginning of this section.

The rest of this manuscript is organized as follows. For the convenience of the reader, section 2 reviews elements of effective techniques for constrained quantum systems. Next, in section 3, the effective semiclassical truncation of a general class of two-component dynamical systems, applicable to homogeneous cosmology, is detailed. In particular, the general construction for switching clocks in such systems is provided. Subsequently, in section 4, we examine in detail the closed FRW model universe minimally coupled to a massive scalar field and, finally, conclude with a discussion and an outlook in section 5.

## 2 Effective equations for constrained quantum systems

The idea behind the effective approach is to avoid operating with specific Hilbert space representations and, instead, to focus on extracting representation independent information. Here we focus on two-component quantum systems with a single constraint that, in addition, plays the role of the Hamiltonian, as is appropriate for homogeneous cosmology with a scalar field providing the matter content. For the purposes of this section, we label the two components by their respective coordinate and momentum operators satisfying the canonical commutation relations

$$[\hat{q}_1, \hat{p}_1] = i\hbar, \quad [\hat{q}_2, \hat{p}_2] = i\hbar.$$

In the effective approach we describe a quantum state through the values it assigns to the four *expectation values*  $\langle \hat{q}_1 \rangle$ ,  $\langle \hat{p}_1 \rangle$ ,  $\langle \hat{q}_2 \rangle$ ,  $\langle \hat{p}_2 \rangle$  and the (countably) infinite set of *moments* [15, 16, 17, 4]

$$\Delta(q_1^{a_1} p_1^{b_1} q_2^{a_2} p_2^{b_2}) := \langle (\hat{q}_1 - \langle \hat{q}_1 \rangle)^{a_1} (\hat{p}_1 - \langle \hat{p}_1 \rangle)^{b_1} (\hat{q}_2 - \langle \hat{q}_2 \rangle)^{a_2} (\hat{p}_2 - \langle \hat{p}_2 \rangle)^{b_2} \rangle_{\text{Weyl}}, \quad (2.1)$$

defined for  $(a_1 + b_1 + a_2 + b_2) \geq 2$ , where the latter quantity will be referred to as the *order* of a given moment. The subscript “Weyl” indicates totally-symmetrized ordering of the product of operators inside the brackets. The space coordinatized by the expectation values and moments

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massive scalar field, to this spatially closed scenario.

<sup>2</sup>Singularity avoidance in this model within the framework of semiclassical gravity was earlier reported in [33].

carries a natural phase space structure defined by the Poisson bracket

$$\{\langle\hat{A}\rangle, \langle\hat{B}\rangle\} = \frac{\langle[\hat{A}, \hat{B}]\rangle}{i\hbar} \quad (2.2)$$

for any pair of operators  $\hat{A}$  and  $\hat{B}$ , extended to the moments using the Leibniz rule and linearity. If there is a true Hamiltonian, it quickly follows from the Heisenberg equation that the evolution of expectation values and moments is generated by the Hamiltonian flow of the quantum Hamiltonian function  $H_Q(\langle\hat{q}_1\rangle, \langle\hat{p}_1\rangle, \langle\hat{q}_2\rangle, \langle\hat{p}_2\rangle; \Delta(\cdots)) = \langle\hat{H}\rangle$  [15, 16].

For a system with a single constraint represented by an operator  $\hat{C}$ , we follow Dirac's constraint quantization condition and demand that physical states satisfy  $\hat{C}|\psi\rangle = 0$ . The analogue of this condition has been formulated directly on the expectation values in [16, 17] as

$$\langle\widehat{pol\hat{C}}\rangle = 0 \quad (2.3)$$

for all polynomials  $\widehat{pol}$  in the four basic variables. Intuitively, this corresponds to eliminating all of the quantum modes involving the constraint operator. The constraint conditions can be systematically imposed by using a linear basis for the polynomial algebra. This leads to an infinite set of constraint conditions on the space of expectation values and moments, which are moreover first-class with respect to the quantum Poisson bracket defined earlier, i.e. the bracket between any two constraint functions vanishes when (2.3) is satisfied [16, 17]. This, in particular, means that the above constraints induce *quantum gauge transformations* on the space of solutions to (2.3) via their Hamiltonian flows. It is easy to see directly from the definition of the quantum Poisson bracket that these flows only affect the expectation values of operators whose quantum commutators with the constraint have a non-vanishing expectation value on the quantum constraint surface; such operators do not correspond to the true physical degrees of freedom of the system (also known as the *Dirac observables*). In this formulation, the search for the physical observables is then replaced by the search for functions of expectation values of polynomial operators, which are invariant along the quantum Poisson flows generated by the constraint functions (2.3) along the constraint surface they define.

Reducing the kinematical system by the action of the constraint is not practically feasible at this step: we are dealing with an infinite dimensional quantum phase space, where we need to impose an infinite set of constraint conditions given by (2.3) and integrate all of the corresponding gauge flows. Fortunately, the system may be approximately represented by a finite number of degrees of freedom in the semiclassical regime with the help of the moments defined above (2.1). Specifying the values of the four expectation values and all of the moments is entirely equivalent to specifying the expectation values of all symmetrized products of the four basic variables: we elect to use the moments as they follow a clear hierarchy when evaluated in a semiclassical state. In particular, we assume that a moment of order  $N$  is of the same semiclassical order as  $\hbar^{N/2}$  and approximate the system by truncating both the degrees of freedom and the system of constraints at some finite order in the semiclassical expansion. This hierarchy is explicitly realized for a class of Gaussian wavefunctions in an ordinary Schrödinger representation of a quantum particle [34] but also holds in a more general class of states. Further details of the effective framework will be explained along the way.

### 3 Leading order quantum corrections and effective dynamics

In the present work we restrict our attention to classical Hamiltonian constraints of the form

$$C_{class} = p_1^2 - p_2^2 - V(q_1, q_2), \quad (3.1)$$

where  $V(q_1, q_2)$  is polynomial, or at least has a convergent power series expansion in  $q_1$  and  $q_2$ . This class of Hamiltonian constraints covers several homogeneous cosmological models one of which is studied in detail in section 4. Since no terms involve products of non-commuting variables, we take the corresponding constraint operator to be

$$\hat{C} = \hat{p}_1^2 - \hat{p}_2^2 - V(\hat{q}_1, \hat{q}_2). \quad (3.2)$$

We systematically impose the constraint conditions (2.3) by demanding

$$\langle \hat{q}_1^a \hat{p}_1^b \hat{q}_2^c \hat{p}_2^d \hat{C} \rangle = 0, \quad (3.3)$$

for all non-negative integer values of  $a, b, c, d$ . We focus on the leading order quantum corrections, which corresponds to truncating the system above semiclassical order  $\hbar$ . Up to this order the kinematics of our system is described by fourteen independent functions: four expectation values of the form  $a = \langle \hat{a} \rangle \propto \hbar^0$ ; four spreads of the form  $(\Delta a)^2 = \langle (\hat{a} - a)^2 \rangle \propto \hbar$  and six covariances of the form  $\Delta(ab) = \langle (\hat{a} - a)(\hat{b} - b) \rangle_{\text{Weyl}} \propto \hbar$ . Note that, due to symmetrization,  $\Delta(ab) = \Delta(ba)$  and  $a$  is used to label both the classical function and the expectation value of the corresponding quantum operator  $\hat{a}$ —it should be clear from the context which of the above it represents. We will use this notation throughout the rest of the present work. After the truncation, five non-trivial independent constraint functions remain (obtained via the substitution  $\hat{a} = a + (\hat{a} - a)$  and Taylor-expanding (3.3) around the expectation values [15, 16, 17, 4])

$$\begin{aligned} C &:= \langle \hat{C} \rangle &= p_1^2 - p_2^2 + (\Delta p_1)^2 - (\Delta p_2)^2 - V - \frac{1}{2} \ddot{V} (\Delta q_1)^2 \\ &&& - \frac{1}{2} V'' (\Delta q_2)^2 - \dot{V}' \Delta(q_1 q_2) \\ C_{q_1} &:= \langle (\hat{q}_1 - q_1) \hat{C} \rangle &= 2p_1 \Delta(q_1 p_1) + i\hbar p_1 - 2p_2 \Delta(q_1 p_2) - \dot{V} (\Delta q_1)^2 - V' \Delta(q_1 q_2) \\ C_{p_1} &:= \langle (\hat{p}_1 - p_1) \hat{C} \rangle &= 2p_1 (\Delta p_1)^2 - 2p_2 \Delta(p_1 p_2) - \dot{V} (\Delta(q_1 p_1) - \frac{1}{2} i\hbar) - V' \Delta(p_1 q_2) \\ C_{q_2} &:= \langle (\hat{q}_2 - q_2) \hat{C} \rangle &= 2p_1 \Delta(p_1 q_2) - 2p_2 \Delta(q_2 p_2) - i\hbar p_2 - \dot{V} \Delta(q_1 q_2) - V' (\Delta q_2)^2 \\ C_{p_2} &:= \langle (\hat{p}_2 - p_2) \hat{C} \rangle &= 2p_1 \Delta(p_1 p_2) - 2p_2 (\Delta p_2)^2 - \dot{V} \Delta(q_1 p_2) - V' (\Delta(q_2 p_2) - \frac{1}{2} i\hbar). \end{aligned} \quad (3.4)$$

Here and from now on we will use the shorthand notation where dots over  $V$  denote partial derivatives with respect to  $q_1$ , primes denote partial derivatives with respect to  $q_2$  and we drop explicit reference to the arguments, so that e.g.  $\dot{V} = \frac{\partial V}{\partial q_1}(q_1, q_2)$ . The system of constraint functions is simple to solve, however the Poisson flows they generate are, in general, difficult to integrate and interpret. The flows have the following general feature: on the constraint surface a non-trivial combination of constraints  $C_{q_1}, C_{p_1}, C_{q_2}, C_{p_2}$  has a vanishing flow. This happens due to the degeneracy of the Poisson structure [15, 16, 17, 4] and is important for the correct reduction in the degrees of freedom. Following the method which was suggested in [16], formalized in [17] and conceptually more thoroughly elucidated in [3, 4], we partially fix the gauge freedom by choosing one of the configuration variables as an internal clock and interpret the single remaining quantum flow as the dynamics. Choosing  $q_1$  as the clock, we impose three ‘ $q_1$ -gauge’ conditions, in order to ‘project the relational clock  $q_1$  to a classical parameter’ [3, 4]

$$\phi_1 := (\Delta q_1)^2 = 0 \quad , \quad \phi_2 := \Delta(q_1 q_2) = 0 \quad , \quad \phi_3 := \Delta(q_1 p_2) = 0. \quad (3.5)$$

In fact, the gauge conditions essentially determine to which Hilbert space representation and clock time slicing (in a deparametrization) the effective relational evolution will correspond [4].<sup>3</sup>

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<sup>3</sup>The quantum phase space, by being *a priori* representation independent, ought to carry the information about a general class of (in general inequivalent) Hilbert space representations based on slicings in a (local) deparametrization (see Sec. IV C in [4] for a detailed discussion).

One gauge flow remains, which preserves both the constraints and the above gauge conditions and is generated by the ‘Hamiltonian’ constraint (see [4] for details on how to obtain  $C_H$ )

$$C_H := C - \frac{1}{2p_1}C_{p_1} - \frac{p_2}{2p_1^2}C_{p_2} - \frac{V'}{4p_1^2}C_{q_2}. \quad (3.6)$$

We solve the constraint functions by eliminating  $p_1$  and the moments generated by  $\hat{p}_1$ . The remaining degrees of freedom are captured by the moments and expectation values of  $\hat{q}_2$  and  $\hat{p}_2$  only, i.e.  $q_2, p_2, (\Delta q_2)^2, \Delta(q_2 p_2), (\Delta p_2)^2$ , as well as the expectation value  $q_1$ . We interpret the resulting system as expectation values and moments generated by the pair  $\hat{q}_2, \hat{p}_2$  evolving relative to the internal clock  $q_1$ , where the corresponding equations of motion are obtained through the Poisson structure (2.2).<sup>4</sup> For consistency of this interpretation we require that the values of these variables satisfy *positivity* conditions

$$\begin{aligned} q_2, p_2, (\Delta q_2)^2, (\Delta p_2)^2, \Delta(q_2 p_2) &\in \mathbb{R} \\ (\Delta p_2)^2, (\Delta q_2)^2 &\geq 0 \\ (\Delta q_2)^2 (\Delta p_2)^2 - (\Delta(q_2 p_2))^2 &\geq \frac{1}{4}\hbar^2 \quad . \end{aligned} \quad (3.7)$$

In [3, 4] it was found that the expectation value of the clock picks up a specific imaginary contribution

$$\Im[q_1] = -\frac{\hbar}{2p_1}, \quad (3.8)$$

in order for the constraint  $C_H$  of (3.6) to be consistently satisfied and for the evolving variables to remain real along the flow generated by it. The real part of  $q_1$  can be used to parametrize the evolution flow, which preserves the above form of the imaginary contribution to  $q_1$ . The gauge-fixing conditions together with the inequalities (3.7) and the interpretation of the remaining flow as the evolution in (the real part of) the internal clock  $q_1$  will from now on be referred to as the *Zeitgeist* associated with  $q_1$ . (Temporally local) relational observables—or *fashionables*—are then given by the correlations of moments and expectation values with the expectation value of the clock and can be interpreted as describing an approximate (local) unitary evolution in  $q_1$  [3, 4]. Notice that these fashionables are state dependent. We can follow an entirely analogous sequence of steps choosing  $q_2$  as the clock, with a minor difference due to the ‘–’ sign in front of  $\hat{p}_2^2$ , yielding a slightly different expression for the new evolution flow generator

$$C_H := C - \frac{1}{2p_2}C_{p_2} - \frac{p_1}{2p_2^2}C_{p_1} + \frac{\dot{V}}{4p_2^2}C_{q_1}. \quad (3.9)$$

The gauge-fixing conditions, imaginary contribution to the clock and positivity conditions are all obtained by simply switching the labels 1 and 2.

Notice that relational evolution in a chosen clock is not only most conveniently interpreted in the corresponding *Zeitgeist*, but, furthermore, in every *Zeitgeist* we evolve a *different* set of relational observables (see [3] and especially Sec. IV C in [4]).

### 3.1 Failure of a *Zeitgeist*, transient observables and transformation to a different clock

For the class of Hamiltonian constraints considered here  $q_1$  is in general not a globally valid clock along the gauge orbits. The breakdown occurs when the evolution rate of the clock

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<sup>4</sup>Expectation values satisfy the classical Poisson brackets (as obvious from (2.2)) and commute with the moments. Furthermore, the Poisson algebra of the moments of two canonical pairs can be found in the appendices of [17, 4]. In this article explicit use is made of this Poisson structure wherever equations of motion are calculated.

becomes very small or vanishes and the clock “reverses direction”. Classically, this happens when  $\{q_1, C_{class}\} = 2p_1 = 0$ , which is possible as  $p_1$  is in general not a constant of motion in these systems. On the effective side, as the expectation value  $p_1$  approaches zero, the  $q_1$ -*Zeitgeist* together with its physical interpretation becomes incompatible with the semiclassical approximation. One can infer this already from the form of the imaginary contribution to the clock (3.8) which becomes divergently large as  $p_1$  approaches zero. Furthermore, the equations of motion for the evolving moments become singular at  $p_1 = 0$  and the moments diverge as they are evolved towards this singularity because the coefficients in the evolution generator (3.6) also diverge as we approach a turning point.

Intuitively, the clock will simply be too slow to resolve the evolution of other degrees of freedom with respect to it when its momentum becomes small (compared to the relevant scale in the system) and thereby lead to large fluctuations in the (relative to  $q_1$  fast) evolving degrees of freedom. These fluctuations/uncertainties must diverge as the clock ‘stops’ (and thus becomes maximally ‘imperfect’). The important consequence is that the quantum evolution in  $q_1$  breaks down *before* the classical turning point and therefore the relational observables in the  $q_1$ -*Zeitgeist* are only locally valid [3, 4]; they are *transient observables*. Notice that the range of validity of the *Zeitgeist* crucially depends on the state.

This is the effective analogue of non-unitarity in  $q_1$  evolution. Indeed, as argued in [4] by analogy with a Schrödinger regime in  $q_1$  internal time, a condition such as  $(\Delta q_1)^2 = 0$  (as required by the  $q_1$ -*Zeitgeist*) is inconsistent in the turning region: violation of unitary evolution would generally result in loss of normalization, so that  $\langle \mathbb{1} \rangle = 1$  will not be preserved leading to a non-zero value for  $(\Delta q_1)^2 = \langle q_1^2 \rangle - \langle q_1 \rangle^2 = q_1^2 (\langle \mathbb{1} \rangle - \langle \mathbb{1} \rangle^2)$ . The clock degree of freedom can thus not be ‘projected to a classical parameter’ anymore and the interference of segments of the wave function before and after the classical turning point causes a mixing of internal time directions, i.e. of positive and negative values of the clock momentum [3, 4]. This conclusion is in agreement with the analysis in [7, 8, 9] where it was shown that a good resolution of relational observables and evolution requires the clock to be essentially decoupled from the other degrees of freedom and its momentum to be large.<sup>5</sup> In this situation one recovers ‘good unitary quantum mechanics’ in both the Schrödinger and Heisenberg picture from the relational dynamics [7, 8]. The state clearly plays a key role in the recovery of an ‘accurately-resolved unitary’ evolution and, in fact, may entirely prevent it if it is highly quantum in nature [7, 9, 3, 4].

Does this indicate that the state is no longer semiclassical past such a turning point? Not necessarily—the semiclassical assumption breaks only relative to a specific set of gauge conditions and the other configuration variable  $q_2$  can serve as a good internal clock near a turning point of  $q_1$ , so long as  $\{q_2, C_{class}\} = -2p_2 \neq 0$ . We can select  $q_2$  as a clock and follow through with the associated gauge fixing and construction of relational observables in a manner entirely analogous to the one employed when choosing  $q_1$  as time. This new  $q_2$ -gauge can eventually also fail, at which point it may be safe to use  $q_1$  as a clock again. It is precisely in order to emphasize this transient nature of the above internal clock frameworks, that we refer to the  $q_1$  gauge and its corresponding dynamical interpretation as the  $q_1$ -*Zeitgeist*. However, if we do not wish to commit to a single clock, we need a method for transferring relational data between the two gauge frameworks.

In order to clarify what would constitute the desired gauge transformation, we begin with a few remarks on the geometry of the situation at hand. The two-component system is described at order  $\hbar$  by fourteen kinematical degrees of freedom. The truncated system of constraints gives five functionally independent conditions  $C_i = 0$  on this space, which therefore restrict the system to a nine-dimensional surface. Five constraint functions, in general, generate four independent flows or vector fields  $X_{C_i}$  on this surface through the Poisson bracket  $X_{C_i}(f) = \{f, C_i\}$ , which

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<sup>5</sup>On the other hand, large energies (or momenta) are an intricate issue in gravitational physics due to black hole forming. Consequently, there is a cap on the clock’s energy and thus on the accuracy of physical clocks [35].

integrate to a four-dimensional gauge orbit. We have introduced three partial gauge-fixing conditions  $\phi_i = 0$ , e.g. (3.5), that break three of the four gauge flows, such that only one independent combination of the vector fields  $X_{C_i}$  preserves the gauge; we interpret this flow as the dynamics in the relevant clock variable. Geometrically, these one-dimensional orbits are formed by the intersection of the surface defined by the gauge conditions  $\phi_i = 0$  with the integral orbits of the set of vector fields  $X_{C_i}$  on the constraint surface. Surfaces corresponding to a different set of gauge conditions  $\phi'_i = 0$  associated with a different internal clock give different one-dimensional intersections with the gauge orbits and, therefore, a different evolution flow. In order to interchange the relational data consistently, we need to go from the  $\phi_i = 0$  surface to the one defined by  $\phi'_i = 0$  without moving off of a given gauge orbit. The most natural way to achieve this is to follow the gauge flows themselves, i.e. to find a combination of the vector fields  $X_{C_i}$  whose integral curve intersects both  $\phi_i = 0$  and  $\phi'_i = 0$ .

Let us be concrete now. Recall, that the  $q_1$ -*Zeitgeist* is given by the conditions  $(\Delta q_1)^2 = \Delta(q_1 q_2) = \Delta(q_1 p_2) = 0$ . The last condition is equivalent to  $\Delta(q_1 p_1) = -i\hbar/2$  if we impose the constraints and the other two gauge conditions, which can be seen directly from  $C_{q_2}$  in (3.4). In this section we will use this alternative form of the third gauge condition for convenience. Similarly, the  $q_2$ -gauge is given by  $(\Delta q_2)^2 = \Delta(q_1 q_2) = \Delta(p_1 q_2) = 0$ , where the last condition is equivalent to  $\Delta(q_2 p_2) = -i\hbar/2$ . To transform from  $q_1$ -gauge to  $q_2$ -gauge we need to find a combination of the vector fields  $G = \sum_i \xi_i X_{C_i}$ , such that a (possibly finite) integral of its flow transforms the variables as

$$\begin{cases} (\Delta q_2)^2 = (\Delta q_2)_0^2 \\ \Delta(q_1 q_2) = 0 \\ \Delta(q_2 p_2) = \Delta(q_2 p_2)_0 \end{cases} \rightarrow \begin{cases} (\Delta q_2)^2 = 0 \\ \Delta(q_1 q_2) = 0 \\ \Delta(q_2 p_2) = -i\hbar/2 \end{cases}, \quad (3.10)$$

where the subscript ‘0’ labels the value of the corresponding variable prior to the gauge transformation.

In general, one would expect such a transformation to be unique up to the dynamical flows of the two ‘Hamiltonian’ constraints in the respective *Zeitgeister*, since they preserve the corresponding sets of gauge conditions. To fix this freedom, and to make the transformation induced on the expectation values small, we fix the multiplicative coefficient of  $X_C$  in  $G$  to zero. There is still some freedom in choosing a path for the gauge transformation: the five constraints generate only four independent flows. Removing  $C$  still leaves us with three independent flows which we can combine. At this point we construct the gauge transformation in two steps. First we search for a flow that satisfies  $G_1(\Delta(q_2 p_2)) = G_1(\Delta(q_1 q_2)) = 0$  on the constraint surface and re-scale the flow such that  $G_1((\Delta q_2)^2) = 1$ . The second step involves finding the flow that satisfies  $G_2((\Delta q_2)^2) = G_2(\Delta(q_1 q_2)) = 0$  and re-scaling this flow such that  $G_2(\Delta(q_2 p_2)) = 1$ . The required gauge transformation will then be given by integrating the flow along  $G = -(\Delta q_2)_0^2 G_1 - (\Delta(q_2 p_2))_0 + i\hbar/2 G_2$ .

The condition  $\Delta(q_1 q_2) = 0$  is shared by both gauge choices and is preserved by  $G$  by construction, we will therefore use this condition to simplify the form of the gauge-transformation fields  $G_1$  and  $G_2$ . The conditions we have imposed determine  $G_1$  and  $G_2$  uniquely and after a number of algebraic manipulations, some of which were performed with the aid of Mathematica 7, one obtains the explicit effect of  $G_1$  and  $G_2$  on the free variables of the  $q_2$ -gauge

$$\begin{aligned} G_1(q_1) &= -\frac{p_1 \dot{V} + 2p_2 V'}{4p_1 p_2^2} & , & \quad G_2(q_1) = -\frac{1}{p_1}, \\ G_1(p_1) &= -\frac{p_1 \ddot{V} + p_2 \dot{V}'}{4p_2^2} & , & \quad G_2(p_1) = 0, \\ G_1(q_2) &= \frac{V'}{4p_2^2} & , & \quad G_2(q_2) = \frac{1}{p_2}, \end{aligned}$$



$$\begin{aligned}
G_1(p_2) &= -\frac{p_1\dot{V}' + p_2V''}{4p_2^2} \quad , \quad G_2(p_2) = 0, \\
G_1((\Delta q_1)^2) &= -\frac{p_1^2}{p_2^2} \quad , \quad G_2((\Delta q_1)^2) = 0, \\
G_1((\Delta p_1)^2) &= -\dot{V}\frac{p_1\dot{V} + 2p_2V'}{4p_1p_2^2} \quad , \quad G_2((\Delta p_1)^2) = -\frac{\dot{V}}{p_1}, \\
G_1(\Delta(q_1p_1)) &= -\frac{p_1\dot{V} + p_2V'}{2p^2} \quad , \quad G_2(\Delta(q_1p_1)) = -1.
\end{aligned}$$

By inspecting (3.10), we infer that, in order to transform between the two gauges, we need to follow the integral curve of the vector field  $G$  for an interval of the flow parameter equal to 1. Denote the flow of  $G$  by  $\alpha_G^s$ , with flow parameter  $s$ . Scalar functions transform via dragging their argument along the flow as  $\alpha_G^s.f(x) = f(\alpha_G^s(x))$ ,  $x \in \mathcal{C}$  where  $\mathcal{C}$  is the constraint surface. The family of translated functions varies differentially along the flow according to the equation

$$\frac{d}{ds}(\alpha_G^s.f)(x) = G(\alpha_G^s.f)(x). \quad (3.11)$$

If  $f(x)$  is smooth along  $G$ , the solution to the above equation can be constructed through the derivative power series

$$\alpha_G^s.f(x) = \sum_{n=0}^{\infty} \frac{s^n}{n!} G^n(f)(x), \quad (3.12)$$

where  $G^n(f)$  is the  $n$ -th derivative of  $f$  along  $G$ , i.e.  $G^n(f) = G(G^{n-1}(f))$  with  $G(f)$  defined as usual.

Here, we are only interested in the transformations to order  $\hbar$ . In our case  $s = 1$  and  $G = aG_1 + bG_2$  where  $a$  and  $b$  are constants of order  $\hbar$ . In addition, for all expectation values and moments  $G_1(f)$  and  $G_2(f)$  are of classical order. It follows, that in the series solution for finite gauge transformations the terms proportional to the second derivative along  $G$  and higher will be of order above  $\hbar$ . We can therefore approximate the gauge transformation to the desired order by the leading order terms, i.e.

$$\alpha_G^1.f(x) = f(x) + G(f)(x) + o(\hbar^2). \quad (3.13)$$

The evolving variables in  $q_2$ -*Zeitgeist* (appearing on the left-hand-side and labeled by the subscript “new”) in terms of those in  $q_1$ -gauge (appearing on the right-hand-side) are given by:

$$\begin{aligned}
q_{1 \text{ new}} &= q_1 + \frac{i\hbar}{2p_1} + \frac{p_1\dot{V} + 2p_2V'}{4p_1p_2^2}(\Delta q_2)^2 + \frac{1}{p_1}\Delta(q_2p_2) \\
q_{2 \text{ new}} &= q_2 - \frac{i\hbar}{2p_2} - \frac{V'}{4p_2^2}(\Delta q_2)^2 - \frac{1}{p_2}\Delta(q_2p_2) \\
p_{1 \text{ new}} &= p_1 + \frac{p_1\ddot{V} + p_2\dot{V}'}{4p_2^2}(\Delta q_2)^2 \\
p_{2 \text{ new}} &= p_2 + \frac{p_1\dot{V}' + p_2V''}{4p_2^2}(\Delta q_2)^2 \\
(\Delta q_1)_{\text{new}}^2 &= \frac{p_1^2}{p_2^2}(\Delta q_2)^2 \\
\Delta(q_1p_1)_{\text{new}} &= \Delta(q_2p_2) + \frac{p_1\dot{V} + p_2V'}{2p_2^2}(\Delta q_2)^2 \\
(\Delta p_1)_{\text{new}}^2 &= \frac{1}{p_1^2p_2^2} \left[ p_2^4(\Delta p_2)^2 + p_2^2(p_1\dot{V} + p_2V')\Delta(q_2p_2) + \frac{1}{4}(p_1\dot{V} + p_2V')^2(\Delta q_2)^2 \right]
\end{aligned} \quad (3.14)$$

All other variables are either gauge-fixed or eliminated using the second order constraint functions  $C_{q_1}, C_{q_2}, C_{p_1}, C_{p_2}$ . The reverse transformation—obtained in an entirely analogous manner—is given by:

$$\begin{aligned}
q_{1 \text{ new}} &= q_1 - \frac{i\hbar}{2p_1} + \frac{\dot{V}}{4p_1^2}(\Delta q_1)^2 - \frac{1}{p_1}\Delta(q_1 p_1) \\
q_{2 \text{ new}} &= q_2 + \frac{i\hbar}{2p_2} - \frac{2p_1\dot{V} + p_2V'}{4p_1^2 p_2}(\Delta q_1)^2 + \frac{1}{p_2}\Delta(q_1 p_1) \\
p_{1 \text{ new}} &= p_1 - \frac{p_1\ddot{V} + p_2\dot{V}'}{4p_1^2}(\Delta q_1)^2 \\
p_{2 \text{ new}} &= p_2 - \frac{p_1\dot{V}' + p_2V''}{4p_1^2}(\Delta q_1)^2 \\
(\Delta q_2)_{\text{new}}^2 &= \frac{p_2^2}{p_1^2}(\Delta q_1)^2 \\
\Delta(q_2 p_2)_{\text{new}} &= \Delta(q_1 p_1) - \frac{p_1\dot{V} + p_2V'}{2p_1^2}(\Delta q_1)^2 \\
(\Delta p_2)_{\text{new}}^2 &= \frac{1}{p_1^2 p_2^2} \left[ p_1^4 (\Delta p_1)^2 - p_1^2 (p_1\dot{V} + p_2V')\Delta(q_1 p_1) + \frac{1}{4}(p_1\dot{V} + p_2V')^2(\Delta q_1)^2 \right]
\end{aligned} \tag{3.15}$$

As expected, the two transformations invert each other up to terms of order  $\hbar^{3/2}$ . It is also straightforward to verify that these gauge transformations preserve, or rather transform, the positivity conditions (3.7). Consider, for example, the transformation from  $q_1$ -*Zeitgeist* to  $q_2$ -*Zeitgeist*, given by (3.14). If the values of the relational observables of the  $q_1$ -gauge satisfy positivity, we can derive the following inequality (see Appendix B of [4])

$$\alpha^2(\Delta q_2)^2 + \beta^2(\Delta p_2)^2 + 2\alpha\beta\Delta(q_2 p_2) \geq 0 \quad , \quad \forall \alpha, \beta \in \mathbb{R} \quad . \tag{3.16}$$

We quickly infer the following for the relational observables of the  $q_2$ -gauge:

- the evolving variables (and thus the relational observables) in the  $q_2$ -*Zeitgeist* are real, while  $q_2$  acquires an imaginary contribution consistent with (3.8);
- $(\Delta q_1)^2 \geq 0$  follows immediately and  $(\Delta p_1)^2 \geq 0$  follows directly from the inequality (3.16);
- the generalized uncertainty relation  $(\Delta q_1)^2(\Delta p_1)^2 - (\Delta(q_1 p_1))^2 \geq \frac{\hbar^2}{4}$  also follows from (3.16) after a few lines of algebra.

Importantly, we see that the gauge transformations are entirely consistent with the imaginary contribution to the expectation value of the clock discussed earlier in this section.

The above construction provides us with the general equations to translate between different *Zeitgeister* in the class of models described by (3.2). Notice that since relational evolution in a given clock choice is best described in its corresponding *Zeitgeist*, a change of clock thus necessitates a change of gauge [4]. As shown in [4], the precise moment of switching between *Zeitgeister* is irrelevant so long as the two *Zeitgeister* are valid before and after the gauge transformation, respectively. The latter condition is crucial and will generally fail in the region of maximal expansion in the cosmological model to be studied in the sequel and thereby cause a breakdown of relational evolution.

## 4 The closed FRW model universe minimally coupled to a massive scalar field

We now wish to extend the scope of the effective framework, described in sections 2 and 3, by applying it to quantum cosmology. We begin by discussing the relevant classical features of the closed FRW model filled with a massive scalar field in section 4.1, proceed by explaining troubles in the quantization of this model in section 4.2 and examine the effective dynamics in detail in section 4.3.

### 4.1 The classical dynamics

The action of a homogenous massive scalar field  $\phi(t)$  minimally coupled to a (homogeneous and isotropic) closed Friedman–Robertson–Walker spacetime, of topology  $\mathbb{R} \times \mathbb{S}^3$  and described by the metric

$$ds^2 = -N^2(t) dt^2 + a^2(t) d\Omega^2 \quad (4.1)$$

(where  $d\Omega^2$  is the line element on a unit  $\mathbb{S}^3$ ), is given by

$$S[a, \phi] = \frac{1}{2} \int dt N a^3 \left( - \left( \frac{1}{aN} \frac{da}{dt} \right)^2 + \frac{1}{a^2} + \left( \frac{1}{N} \frac{d\phi}{dt} \right)^2 - m^2 \phi^2 \right) . \quad (4.2)$$

Variation of the action with respect to lapse  $N$ , field  $\phi$  and scale factor  $a$  yields the Friedman–, ‘Klein–Gordon’– and Raychaudhuri–equation, respectively, ( $\dot{\phantom{x}} = N^{-1} \frac{d}{dt}$ )

$$\dot{a}^2 = -1 + a^2 \left( \dot{\phi}^2 + m^2 \phi^2 \right) , \quad (4.3)$$

$$\ddot{\phi} + \frac{3\dot{a}}{a} \dot{\phi} + m^2 \phi = 0 , \quad (4.4)$$

$$\ddot{a} = a \left( m^2 \phi^2 - 2\dot{\phi}^2 \right) . \quad (4.5)$$

These equations of motion are clearly not all independent (e.g., differentiating (4.3) and combining it with (4.4) gives the Raychaudhuri–equation (4.5)).

Despite the apparent simplicity, the model possesses a surprisingly rich solution space [20, 22, 23, 25, 26, 27, 28]. We do not intend to review the details here, but wish to summarize and pinpoint those classical aspects which are essential for our subsequent discussion in the quantum theory.

This model universe attracted significant interest, mainly because the mass–term of the scalar field can act as an ‘effective cosmological constant’ in certain regimes and thereby drive a deSitter–type inflationary period. Indeed, various phases of cosmological evolution are possible because the equation of state of the scalar field itself varies throughout evolution [25, 36]. In [25] it was shown, using methods of dynamical systems, that inflationary stages are a ‘generic’ property of solutions to (4.3, 4.4). Setting initial conditions at some small value of the scale factor, the scalar field  $\phi(t)$  decreases with increasing  $a$ , generating an inflationary phase, and subsequently evolving to its equilibrium value  $\phi \approx 0$  around which the field begins to oscillate<sup>6</sup> with frequency  $m$  and the model universe exhibits a matter–dominated era in which  $a \propto t^{2/3}$  [20, 22, 23, 24, 25]. (The inflationary period is longer for larger initial values  $\phi_0$  of the scalar field [20].) Thereupon the scale factor can begin to oscillate between points of regular (non–global) maxima  $a_{max,k}$  and (non–global) minima  $a_{min,k}$  [22, 23, 25, 26]. A generic solution will evolve to

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<sup>6</sup>As discussed in [24, 21] a solution which expands out to a length scale of the order of  $10^{60}$  Planck lengths requires at least  $10^{60}$  such oscillations of  $\phi$ .

a point of maximum extension—the turning point— $a_{max}$  (possibly oscillate around this point a few times) and eventually recollapse to a big crunch singularity [20, 22, 25]. Thus, clearly, both  $\phi$  and  $a$  will generically fail to be globally valid internal clock functions in this model.<sup>7</sup> Two typical classical solutions are displayed in figure 1.

In fact, the situation for relational evolution appears even worse: as noted in [22, 20, 21, 25, 28], there exists a countably infinite discrete set of periodic solutions which bounce without ever encountering a spacetime singularity. In [22, 26, 28], furthermore, it was shown that even an uncountably infinite discrete set of perpetually bouncing aperiodic solutions (of measure zero in the space of solutions [27, 28]) exists which exhibits an interesting fractal-like behavior. The system (4.3, 4.4) is thus non-integrable and chaotic [22, 26, 28]; this feature lies at the root of many troubles in the quantum theory.

The reason for the absence of a globally valid internal clock function in this model universe can be seen especially nicely in the Hamiltonian formulation which is required anyway in order to compare with the effective results in section 4.3 below. For practical purposes, let us perform a variable transformation  $\alpha = \ln(a)$  and henceforth work with  $\alpha$ . This is convenient as, first, in the quantum theory one thereby avoids a factor ordering problem in the Hamiltonian constraint [2, 24] (see (4.13) below), second, the resulting quantum Hamiltonian constraint (4.13) is explicitly of the form (3.2) and thus the effective constructions of section 3 are directly applicable, and, third, we now have  $-\infty < \alpha < \infty$  and  $-\infty < \phi < \infty$  and thus a configuration space  $\mathcal{Q} = \mathbb{R}^2$  which is somewhat simpler to quantize than  $\mathcal{Q} = \mathbb{R} \times \mathbb{R}_+$  [2, 37].<sup>8</sup> The big bang and big crunch singularities will now appear at  $\alpha \rightarrow -\infty$  which is not an issue for our purposes since in the effective approach we shall be focussing on the regime of maximal expansion of the scale factor  $a$  (presumably, only a full quantization can cope with the classically singular regime, however, see [31]). For completeness, note, furthermore, that when discussing the quantum dynamics in sections 4.2 and 4.3 below, small (big) fluctuations in  $\alpha$  do not necessarily translate into small (big) fluctuations in  $a$ .

Choosing a gauge  $N = e^{3\alpha}$ , it is straightforward to arrive at the expression for the Hamiltonian constraint corresponding to the system (4.2) [24, 38]

$$C_H = p_\phi^2 - p_\alpha^2 - e^{4\alpha} + m^2 \phi^2 e^{6\alpha} = 0 \quad , \quad (4.6)$$

which is precisely of the form (3.1). The term  $m^2 \phi^2 e^{6\alpha}$  provides the coupling between the relational clock, i.e. either  $\alpha$  or  $\phi$ , and the evolving configuration variable, i.e. either  $\phi$  or  $\alpha$ , respectively. In fact, the squared mass  $m^2$  can be interpreted as the coupling constant, while the factor  $e^{6\alpha}$  can in certain regimes be treated as an adiabatic factor [7, 24]. This coupling term will have a great effect on quantum relational evolution. Using the symplectic structure on  $T^*\mathcal{Q}$ , the corresponding canonical equations of motion read

$$\begin{aligned} \dot{\alpha} &= \{\alpha, C_H\} = -2p_\alpha \quad , \\ \dot{p}_\alpha &= \{p_\alpha, C_H\} = 4e^{4\alpha} - 6m^2 \phi^2 e^{6\alpha} \quad , \\ \dot{\phi} &= \{\phi, C_H\} = 2p_\phi \quad , \\ \dot{p}_\phi &= \{p_\phi, C_H\} = -2m^2 \phi e^{6\alpha} \quad , \end{aligned} \quad (4.7)$$

where now the overdot refers to differentiation with respect to the coordinate time  $t$ . As a consequence of  $N = e^{3\alpha}$ , note that henceforth  $t$  does *not* coincide with the proper times  $\tau$  of

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<sup>7</sup>For small masses  $m$ , the scalar field  $\phi(t)$  is still a monotonically increasing function of  $t$  as in the massless case and thus a good global clock (see also the discussion in [26], in particular, the region in configuration space called ‘region 0’).

<sup>8</sup>For instance,  $\hat{p}_a$  is *not* self-adjoint on  $L^2(\mathbb{R}_+, da)$ . Or, when choosing  $L^2(\mathbb{R}, da)$  instead, one would somehow have to give meaning to  $a < 0$ . On the other hand,  $\hat{p}_\alpha$  is self-adjoint on  $L^2(\mathbb{R}, d\alpha)$  and  $-\infty < \alpha < +\infty$ .

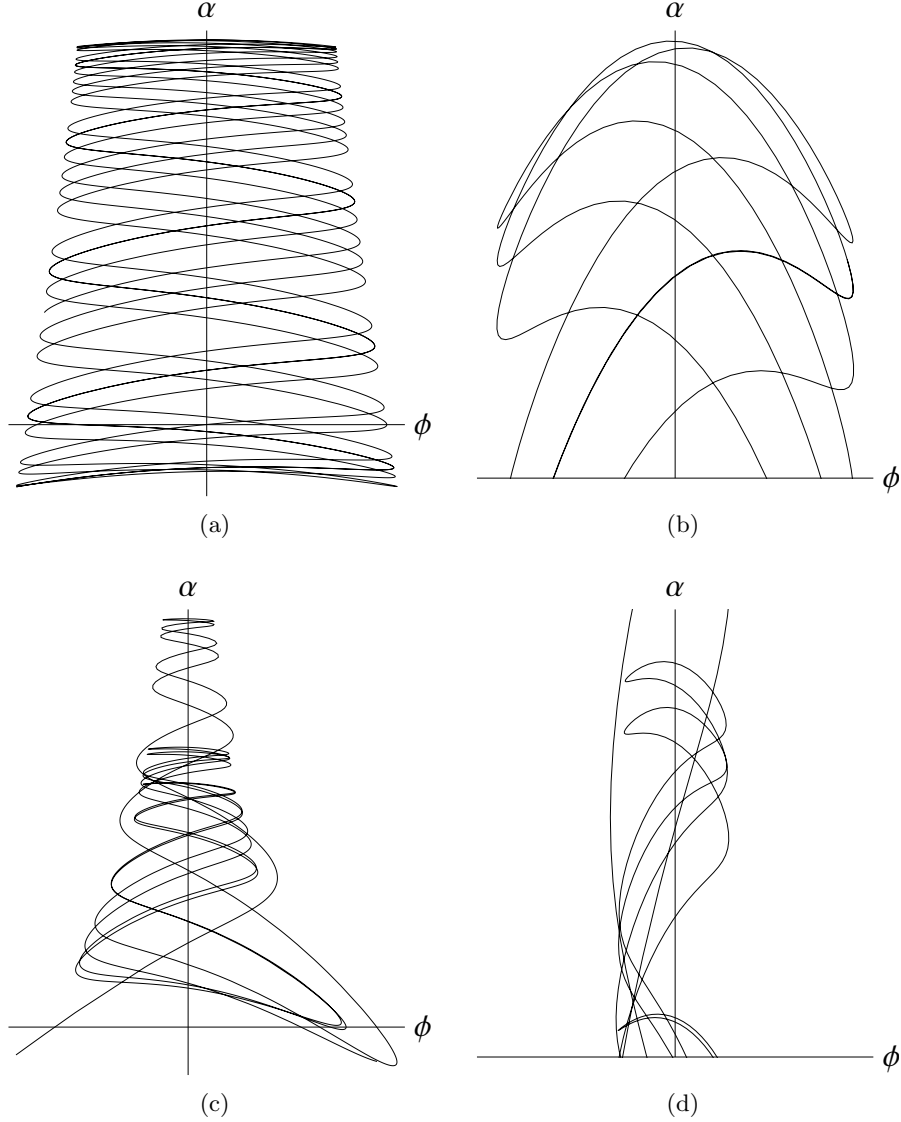


Figure 1: Two typical classical solutions to the closed FRW spacetime—both  $\phi$  and  $a$  generically fail to be globally valid internal clock functions in this model. Here we used  $\alpha = \ln(a)$  as appropriate for the canonical discussion following (4.6, 4.7). (a) and (c) show extended segments of (both the expanding and re-contracting branch of) relational evolution up to the point of maximal expansion  $\alpha_{max} = \ln(a_{max})$ . The (new) scale factor  $\alpha$  oscillates between points of regular (non-global) maxima  $\alpha_{max,k} = \ln(a_{max,k})$  and (non-global) minima  $\alpha_{min,k} = \ln(a_{min,k})$ ; (b) shows a close-up of the same configuration space trajectory as (a) near  $\alpha_{max}$ , displaying the non-global extrema in a greater detail, while (d) depicts a close-up on an intermediate section of the trajectory in (c).

comoving observers in (4.1). Figure 2 depicts the behavior of the canonical variables for a rather benign solution.

In a work concerning the precise origin of non-unitary relational evolution in the quantum theory of finite-dimensional parametrized systems [38], Hájíček, in fact, has shown that unitarity requires the existence of a (temporally) global internal clock function already at the classical level which, in turn, was shown to be equivalent to the classical system being reducible. As an example, the system governed by (4.2, 4.6) was considered and it was shown that [38]:

1. the constraint surface  $\mathcal{C}$  defined by (4.6) in  $T^*\mathcal{Q}$  is of topology  $\mathcal{C} = \mathbb{R}^2 \times \mathbb{S}^1$  and thus connected but not simply connected, and
2. the flow of  $C_H$  on  $\mathcal{C}$  has no critical points, but incontractible cycles (around  $\mathbb{S}^1$ ).

The incontractible cycles, of course, correspond to the periodically bouncing solutions [20, 22, 26, 28] alluded to above. These cycles of the Hamiltonian flow on  $\mathcal{C}$  prevent the system from being (globally) reducible and possessing a global clock [38].

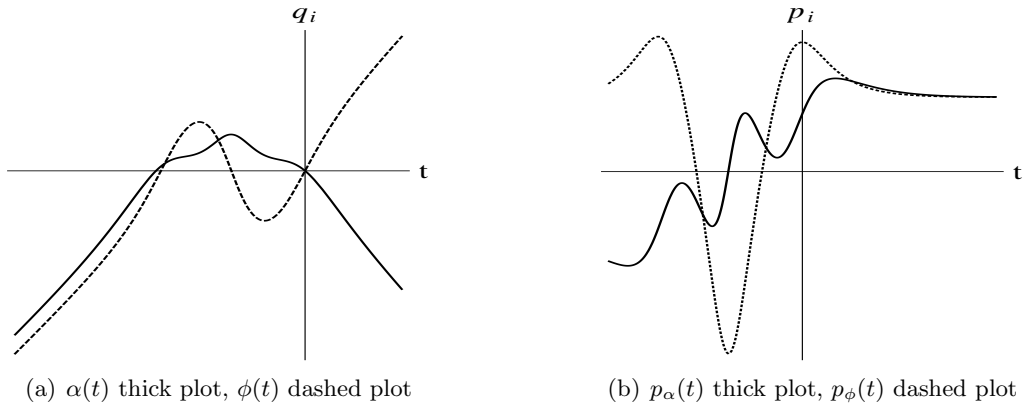


Figure 2: Evolution of the canonical variables governed by (4.7) for a rather benign classical solution. Notice how  $\alpha$  features quasi-turning points closely to the turning points of  $\phi$  (also manifested in  $p_\alpha$  having a local minimum close to the zeros of  $p_\phi$ ).

#### 4.1.1 Classical relational dynamics and non-integrability

Let us make a few statements regarding relational evolution in this non-integrable model universe. This is of relevance, because in the majority of the literature on relational dynamics the possibility of non-integrability, despite it being a typical property of generic dynamical systems [14] and having severe repercussions for relational evolution, is largely ignored. We therefore believe that the results of the present article are a first step towards a more general discussion of the fate of relational dynamics, specifically in the quantum theory. In particular, non-integrability means that the system does not possess any global constants of motion (i.e. Dirac observables) other than the Hamiltonian itself [14].<sup>9</sup> Nevertheless, relational evolution and Dirac observables may still exist *locally* (in ‘time’), or rather implicitly and by means of the implicit function theorem one could, in principle, still explicitly derive locally valid observables.<sup>10</sup> This, certainly, features in the quantum theory and this is where we expect the effective

<sup>9</sup>In fact, in the present model the Hamiltonian constraint (4.6) coincides with the first integral of motion defined by the Friedman-equation (4.3).

<sup>10</sup>For instance, in Eq. (5.6) of [24] the relational observable  $\phi(a)$  is given for the matter dominated phase of expansion where  $a \propto \tau^{2/3}$  and  $\tau$  is proper time.

approach to relational evolution [3, 4] to come in handy as it enables one to make sense of local time evolution and (temporally) local relational observables (aka *fashionables* in the terminology of [3, 4]) in the semiclassical regime. However, even if locally a complete set of relational observables is derived—in contrast to integrable systems—this set in general no longer characterizes the orbit because chaotic systems typically possess ergodic orbits which come arbitrarily close to any point on the energy surface (i.e., for constrained systems the constraint surface) [14].

Another generic—and related—property of chaotic systems is the instability of initial data [14]: chaotic systems generally contain closed (periodic or unperiodic) orbits which are unstable in the sense that a trajectory based on initial data arbitrarily close to such a closed orbit will typically exponentially diverge from the closed orbit and eventually become entirely uncorrelated.<sup>11</sup> The closed orbits of the present model universe were described in detail in [22, 26, 28]. In particular, in [28] the resulting fractal structure in the space of initial data was nicely exhibited, demonstrating how solutions initially arbitrarily close can experience completely unrelated fates. In fact, defocussing of nearby trajectories occurs in the present model also for trajectories not arbitrarily close to a closed orbit. For instance, figure 3 depicts how neighboring trajectories fan out in the region of maximal expansion already for a rather well-behaved classical solution. For generic solutions exhibiting more oscillations in both  $\phi$  and  $\alpha$  [26], this feature will get more pronounced. Such defocussing will be particularly relevant in the quantum theory, since it constitutes the ultimate cause of a generic breakdown of semiclassicality and relational evolution.

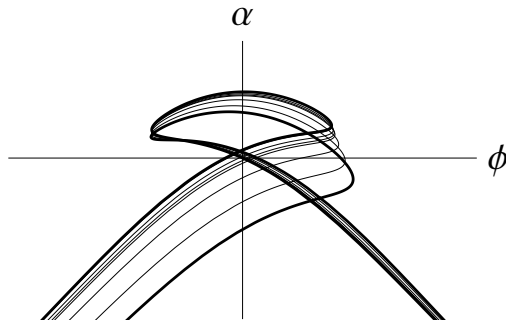


Figure 3: Defocussing of nearby trajectories, caustics develop along the extrema of  $\phi$  (see also [23]).

Finally, classically there is no obstruction to using either  $\alpha$  or  $\phi$  as a global clock function despite the turning points of the clock variables and the ensuing multi-valuedness of the relational observables, because we can always resort to the gauge parameter in order to provide an ordering to the correlations [4]. Nevertheless, it is more practical to employ  $\alpha$  as an internal clock for large parts of the evolution due to the highly oscillatory nature of the scalar field at large volumes. In the quantum theory, it will no longer be possible to employ either variable globally due to non-unitarity and a break down of evolution *before* classical turning points.

Classically, one imposes suitable (compatible with  $C_H$ ) initial data at some fixed  $t = t_0$ , which can be translated into a relational initial value problem (IVP): when using  $\alpha$  as clock, one could choose  $\phi(\alpha_0)$  and  $p_\phi(\alpha_0)$  at some value  $\alpha_0 = \alpha(t_0)$ , which, of course, corresponds to a point in phase space, for instance, some configuration on the expanding branch of cosmic evolution, if one chooses the (here due to (4.7)) negative sign solution for the initial clock momentum,  $p_\alpha(t_0)$ , via the constraint (4.6). Indeed, in relativistic systems subject to constraints quadratic in the

<sup>11</sup>Clearly, such a statement depends strongly on the time coordinate which is potentially dangerous in general relativity, however, there exists a very general definition of chaotic behavior which takes this into account and essentially requires a defocussing of trajectories (i.e. no statement is made about how rapid the defocussing occurs), as well as ergodicity [39].

momenta, a relational IVP additionally requires an initial internal time direction in order to relationally evolve [4, 40]. The data is subsequently evolved through the maximal extension into the big crunch singularity, such that the contracting branch is classically the logical successor of the expanding branch. In contrast to earlier work [5, 24, 30] on the quantum theory of (4.2), we shall perform the same IVP construction for sufficiently semiclassical states in the effective framework in section 4.3 below.

## 4.2 Troubles for Hilbert space quantizations

The classical non-integrability of the model suggests a rather complicated quantum dynamics. Indeed, generally the transition from quantum to classical is a highly non-trivial challenge in chaotic models and qualitatively quite distinct from the analogous task for non-chaotic systems [14]. While substantial research has been devoted to gaining a general (but mostly approximate) understanding of at least the semiclassical solutions to the present model in various approaches [20, 21, 23, 24, 30, 31, 33], dynamical (relational) questions have thus far not been properly addressed. This is simply because no (non-trivial) exact quantum solutions are known, let alone a physical inner product on the space of solutions in which one could compute expectation values of various quantities. In order to be able to compare with the effective relational dynamics of section 4.3, we ideally would like to extract (at least approximate) dynamical information from the Hilbert space or path-integral quantizations carried out thus far. In the present section, we wish to explain why it is practically difficult to extract relational dynamics from any of the previous approaches.

To this end, we firstly recall a result presented in [4]: the effective relational dynamics in a toy model devoid of global clocks was shown to be equivalent at order  $\hbar$  to the dynamics (of expectation values) in a (temporally) local internal time Schrödinger regime. The latter is obtained by a local deparametrization of the classical model and a subsequent quantization. For a model governed by a quadratic constraint of the form  $C = p_t^2 - H^2(t, q, p)$ , one can locally deparametrize by choosing a local clock, say,  $t$  and factorizing the constraint as  $C = C_+ C_- = (p_t + H)(p_t - H)$ . Standard quantization of  $C_\pm$  yields a Schrödinger equation with ‘time-dependent’ square-root Hamiltonian  $\hat{H}$  (defined by spectral decomposition)

$$i\hbar\partial_t\psi(t, q) = \pm\hat{H}(t, \hat{q}, p)\psi(t, q), \quad (4.8)$$

which, if  $t$  is a non-global internal clock, is only locally valid (in ‘time’  $t$ ) because of non-unitarity. One may thus wonder whether a similar construction could be performed for the present model universe such that we may compare the local dynamics of the Schrödinger regime with the effective results. In fact, this question was already considered (for very different reasons) in an early work on quantum cosmology by Blyth and Isham [41], in which they investigated a reduced quantization of FRW models filled with a homogenous scalar field. They considered various choices of relational time variables (chosen before quantization) which all yield distinct time-dependent Schrödinger equations with square-root Hamiltonians that describe precisely the desired Schrödinger regimes.<sup>12</sup> As regards the relation between the Schrödinger regime and a Dirac quantization yielding a Wheeler–DeWitt (WDW) equation (with quantized  $\hat{t}$ ),

$$\hat{H}^2(\hat{t}, \hat{q}, \hat{p})\tilde{\psi}(q, t) = \hat{p}_t^2\tilde{\psi}(q, t) = -\hbar^2\partial_t^2\tilde{\psi}(q, t), \quad (4.9)$$

it was noted in [41] that (4.9) does *not* follow from (4.8) when  $\hat{H}$  is explicitly time dependent, because acting with  $\pm\hat{H}$  on both sides of (4.8)—rather than (4.9)—yields

$$\hat{H}^2(t, \hat{q}, \hat{p})\psi(t, q) = -\left(\hbar^2\partial_t^2 \pm i\hbar\partial_t\hat{H}(t, \hat{q}, \hat{p})\right)\psi(t, q). \quad (4.10)$$

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<sup>12</sup>One of the motivations of [41] to quantize by the reduction procedure, instead of a Dirac quantization leading to a Wheeler–DeWitt equation was to avoid the non-positive definiteness of Klein–Gordon type inner products.



However, in [3] it was shown that to *order*  $\hbar$  the expectation value versions<sup>13</sup> of (4.8) and (4.9) *are*, in fact, solved by the *same* state  $\psi = \tilde{\psi}$  if the expectation value of the ‘internal time operator’  $\hat{t}$  in (4.9) is complex with imaginary part coinciding with the effective result (3.8)

$$\Im[\langle \hat{t} \rangle] = -\frac{\hbar}{2\langle \hat{p}_t \rangle}. \quad (4.11)$$

To semiclassical order, the Schrödinger regime may thus be understood as locally approximating a solution to the relativistic WDW equation (away from classical turning points).

However, the explicit construction of solutions in [41] was only carried out for the  $k = 1$ ,  $m = 0$  and for the  $k \leq 0$ ,  $m \neq 0$  FRW models. The reason for avoiding the present model is explained as follows: in our case (4.6), the classical Hamiltonian for evolution in  $t = \alpha$  time is given by  $H(\alpha; \phi, p_\phi) = \sqrt{p_\phi^2 - e^{4\alpha} + m^2 \phi^2 e^{6\alpha}}$ , while the one for evolution in  $t = \phi$  time reads  $H(\phi; \alpha, p_\alpha) = \sqrt{p_\alpha^2 + e^{4\alpha} - m^2 \phi^2 e^{6\alpha}}$ . The ensuing quantum Hamiltonian  $\hat{H}(t, \dots)$  is not only ‘time-dependent’ but also fails to commute with itself at different ‘times’,  $[\hat{H}(t, \dots), \hat{H}(t', \dots)] \neq 0$  for both  $t = \alpha, \phi$ . Consequently, ‘energy’ eigenstates at a given ‘time’ fail to be eigenstates at later ‘times’ and the formal solution to (4.8) involves a Dyson time-ordering

$$\psi(t, q) = \hat{U}(t, t_0) \psi(t_0, q) = T \left[ \exp \left( \mp \frac{i}{\hbar} \int_{t_0}^t \hat{H}(s, \hat{q}, \hat{p}) ds \right) \right] \psi(t_0, q). \quad (4.12)$$

Constructing explicitly the time-evolution operator  $\hat{U}(t, t_0)$  with either  $\hat{H}(\alpha; \hat{\phi}, \hat{p}_\phi)$  or  $\hat{H}(\phi; \hat{\alpha}, \hat{p}_\alpha)$ , unfortunately, does not (even to order  $\hbar$ ) seem feasible for this non-integrable system. We thus abstain from further attempting to construct a local Schrödinger regime.

Next, in order to extract relational dynamics from the quantum theory, one could try to solve the WDW equation and consider a suitable inner product in order to compute expectation values which may be compared to the effective results. The canonical Dirac quantization was considered, e.g., in [23, 24, 30]. The standard quantization of (4.6) yields a Klein–Gordon type hyperbolic partial differential equation (setting for now  $\hbar = 1$ ),<sup>14</sup>

$$\left( \frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial \phi^2} - e^{4\alpha} + m^2 \phi^2 e^{6\alpha} \right) \psi(\alpha, \phi) = 0, \quad (4.13)$$

with variable mass  $M^2 = e^{4\alpha}(e^{2\alpha}m^2\phi^2 - 1)$  in the 2D Lorentzian superspace metric

$$ds^2 = -d\alpha^2 + d\phi^2. \quad (4.14)$$

Thus,  $\alpha = \text{const}$  is a ‘spacelike’ slice in minisuperspace.

WKB approximations to this equation have been extensively studied, e.g., in [24, 20, 23, 28, 29] from various perspectives, all reporting a breakdown of this semiclassical expansion in the region of maximal extension. A WKB approximation  $\psi = \sum_n C_n(\alpha, \phi) \exp(\pm i S_n(\alpha, \phi))$  is valid only if the amplitude  $C_n$  varies much slower than the phase  $S_n$  [42, 29, 20, 24, 23]. As pointed out in [28, 23], the caustics resulting from focussing of nearby classical trajectories (see also figure 3 above) cause  $|C_n|^2 \rightarrow \infty$ , while  $|C_n|^2$  goes rapidly to zero where classical trajectories defocus, for instance, in the region of maximal expansion also in figure 3, which leads to a generic breakdown of the WKB approximation. This is of relevance for an at least qualitative comparison to the effective results displayed in section 4.3 below. Consequently, we wish to summarize the pivotal features of previous semiclassical constructions.

<sup>13</sup> Assuming a standard  $t = \text{const}$  Schrödinger theory inner product away from any turning points.

<sup>14</sup> Note that the choice of variables (and in this case trivial) factor ordering here is such that the derivative terms constitute the invariant d’Alembertian with respect to the minisuperspace metric (4.14).

For instance, Kiefer [24] imposed initial data for  $\psi$  on a ‘spacelike’ slice  $\alpha = \text{const}$  in order to construct wave packets in minisuperspace, approximately solving (4.13) via a Born–Oppenheimer (with expansion parameter  $m_p^{-1}$ ) and a subsequent WKB approximation. Tubelike standing waves representing classically expanding and contracting universes could be constructed if an additional ‘final condition’ in  $\alpha$ , namely  $\psi \rightarrow 0$  as  $\alpha \rightarrow \infty$ , was imposed for reasons of ‘normalizability’.<sup>15</sup> The turning point  $\alpha_{\text{max}}(n)$  of the individual oscillator modes in the wave packet depends strongly on the mode  $n$  and thus the reflection of the wave packet at the average  $\alpha_{\text{max}} = \alpha_{\text{max}}(\bar{n})$  is described by a (chaotic) scattering phase shift which depends on the mass and is a multiple of  $\pi$  only for discrete values of  $m$  [24]. Narrow wave tubes on both the expanding and re–contracting branch can thus only be constructed for these special values of  $m$  and only away from the classical turning region, i.e. only for  $\alpha \ll \alpha_{\text{max}}$ . Furthermore, Hawking applied the ‘no–boundary–proposal’ [43] (which renders an IVP superfluous) to the present model [20]. The ensuing (semiclassical) wave function can be interpreted as a superposition of quantum states peaked around an ensemble of non–singular bouncing solutions with long inflationary period which correspond to the aforementioned set of measure zero periodic and aperiodic solutions [22, 26, 28].<sup>16</sup> Numerical evidence for these results was exhibited in [21], while similar outcomes with, however, special attention to singular classical trajectories were reported in [29]. Page [23] approximated the Hawking wave function by starting from the canonical constraint (4.13) and translating the ‘no–boundary–condition’ into sufficient Cauchy data. Also this WKB approximation breaks down due to caustics at the extrema of  $\phi$  [23].

As regards the classical determinism, mentioned in section 4.1.1, of having the re–contracting branch as the logical successor of the expanding one, it was maintained in [5, 24, 30] that:

- (1) The quantum IVP is very different from that in the classical theory. Initial data has to be imposed on *all* of the minisuperspace–slice  $\alpha = \text{const}$ , implying that both branches have to be there ‘initially’ (in  $\alpha$ ). ‘Initial’ and ‘final state’ can no longer be distinguished.
- (2) It is meaningless in quantum cosmology to extend classical paths through the turning region of  $\alpha$  into the re–collapsing phase. The WKB approximation does not provide the complete classical trajectory. The latter could only be obtained through continuous measurement by higher degrees of freedom (which would suppress the scattering at  $\alpha_{\text{max}}$ ).

However, these statements partially depend on the construction used in [24], namely, (a), on obtaining the semiclassical limit by means of a WKB approximation, (b), on using solely  $\alpha$ , rather than  $\phi$ , as the internal clock and, (c), on the ‘final condition’,  $\psi \rightarrow 0$  as  $\alpha \rightarrow \infty$ . Let us discuss this point for point.

(a) While a WKB approximation is one way of obtaining semiclassical information from a quantum model, it is not the most general semiclassical approximation and necessarily breaks down for chaotic systems [28]. On the other hand, the semiclassical approximation employed in the effective approach is very general in nature. We shall see in section 4.3 that semiclassicality *can* be achieved in the classical turning region, however, only for sufficiently peaked initial effective states. A fairly classical trajectory with the re–collapsing branch being the logical successor of the expanding one can thus be obtained *without* decoherence of additional degrees of freedom.

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<sup>15</sup>While sensible in the construction of [24], the ‘final condition’ should not be viewed as a ‘normalization condition’ because normalization requires an inner product. In fact, in [23] no ‘final condition’ was imposed and the wave function not strongly damped for large  $\alpha$  which was interpreted as leading to a high probability that the universe would be large compared to the Planck length. (Although a probabilistic interpretation, again, requires a consistent inner product which, as discussed below, awaits identification.)

<sup>16</sup>This is in agreement with standard results on the semiclassical limit of quantum models which are classically chaotic. Semiclassical states are typically concentrated on the closed orbits of measure zero [14].

(b) The (chaotic) scattering of the wave packet around  $\alpha_{max}$  [24, 30] manifests non-unitarity in  $\alpha$  evolution. Indeed, as pointed out in [3], the interference of segments of the wave function/packet before and after the turning region of a non-global internal time function—as a result of different modes having different turning points—leads to a superposition of (internal) time directions, i.e. of positive and negative frequencies associated to the spectrum of the momentum conjugate to the internal clock function. This necessarily leads to a breakdown of the evolution in the non-global clock and of inner products based on its level surfaces *before* the classical turning point. This is in agreement with the analysis in [7] concerning the reconstruction of the unitary Schrödinger and Heisenberg picture from relational quantum dynamics which turns out to be only locally feasible for sufficiently semiclassical states and clock degrees of freedom far enough away from any clock turning points. Unitarity in a given time variable is tantamount to preservation of such inner products in the evolution with respect to the time variable which is evidently not possible here. Instead, one could switch to relational evolution in a new clock if it behaves sufficiently ‘semiclassically’ in the turning region of the first clock [3, 4]. If no such degree of freedom is admitted by the state, relational evolution necessarily breaks down. In the present model universe,  $\phi$  may be used for sufficiently benign and semiclassical states as an intermediate clock in the turning region of  $\alpha$ . Whereas it is not clear how this could be achieved at the level of the WDW equation, this is precisely what will be carried out in the effective framework in section 4.3. At the effective level, the non-local IVP and single evolution generator of [5, 24, 30] is traded for a local IVP solely imposed, say, on the expanding branch and for the necessity of two evolution generators, one in  $\alpha$ , the other in  $\phi$  time.

(c) In fact, it is the ‘final condition’ which prevents narrow wave packets around  $\alpha_{max}$ ; only exponentially (in  $\alpha$ ) decreasing modes are allowed and the data for both the expanding and re-contracting branch must be present initially at  $\alpha_0$ , however, is subsequently scattered at  $\alpha_{max}$  [24, 30, 5]. On the other hand, no final condition can be imposed in the effective approach which for sufficiently benign states, nonetheless, yields semiclassical trajectories in the region of maximal expansion.

Let us consider (naïve) possibilities for an inner product. (i) Since the operator  $\hat{H}^2 = -\partial_\phi^2 - e^{4\alpha} + m^2\phi^2 e^{6\alpha}$  is not generally non-negative, evolution with respect to  $\alpha$  is non-unitary and a standard Schrödinger type inner product clearly not preserved. (ii) Group averaging [44] is commonly employed in constructing physical inner products in quantum cosmology, however, requires integrating over the flow of the quantum constraint which does not seem practical on account of the classical non-integrability. (iii) There exists a method going back to DeWitt [40, 45] which yields a conserved quadratic form on  $\mathcal{H}_{phys}$  from  $\mathcal{H}_{aux}$  which in the present case is just  $L^2(\mathbb{R}^2, d\alpha d\phi)$ :

**Theorem 4.1.** *Let  $(Q, \eta)$  be an  $n$ -dimensional configuration manifold with volume form  $\eta$ , and  $\hat{C}$  be a second-order differential operator on  $\mathcal{C}_0^2(Q, \mathbb{C})$  (space of twice differentiable complex functions with compact support on  $Q$ ) that is symmetric with respect to the scalar product on  $L^2(Q, \eta)$ . Then, for any  $\Psi, \Phi \in \mathcal{C}_0^2(Q, \mathbb{C})$ , there is a vector field  $\vec{J}[\Psi, \Phi]$  on  $Q$  such that*

$$(\hat{C}\Psi)^*\Phi - \Psi^*(\hat{C}\Phi) = \text{Div}_\eta \vec{J}. \quad (4.15)$$

Clearly, if both  $\Psi, \Phi$  are annihilated by a hyperbolic  $\hat{C}$ ,  $\vec{J}$  defines a conserved current on the space of solutions to  $\hat{C}\psi = 0$ . It is not difficult to convince oneself, that for the constraint (4.13)  $\vec{J}$  is just given by the standard Klein–Gordon current vector,

$$J^a = g^{ab}[(\partial_a \Psi^*)\Phi - \Psi^*(\partial_a \Phi)], \quad (4.16)$$

where  $g^{ab}$  is the inverse 2D minisuperspace metric (4.14), such that the conserved quadratic form provided by the theorem coincides with the Klein–Gordon inner product. Unlike in the

case of a Klein–Gordon particle, we cannot restrict ourselves here globally to positive or negative frequency modes (on whose subspaces the Klein–Gordon inner product would be positive definite), because no global clock exists and ‘positive’ and ‘negative frequencies’ in  $\alpha$  time will necessarily mix up in the turning region of  $\alpha$ . In addition, the Klein–Gordon charge is identically zero for real  $\Psi, \Phi$  and thereby trivially conserved. The semiclassical (approximate) solutions of [20, 21, 23, 24] are real. Hence, it is not even possible to use the Klein–Gordon inner product as an approximation for known semiclassical states on only the ‘negative’ (i.e. expanding) or ‘positive frequency’ (i.e. re-collapsing) branch away from the turning region in which frequencies mix up. It, therefore, remains unclear what the correct physical inner product should be and how the *Hilbert space problem* could be solved.

In conclusion, relational dynamics of this non-integrable model seems currently only practically feasible in the effective approach (and also there only in a limited regime) since it sidesteps many technical difficulties associated to a Hilbert space quantization [4].

### 4.3 Effective relational dynamics

Following the general procedure laid down in sections 2 and 3, we now turn to the effective treatment of the closed FRW model. Since we are only interested in the semiclassical regime, we need not solve the full quantum dynamics but only ‘expand around’ classical trajectories. The non-integrability is hence not a *technical* problem for us when studying semiclassical states corresponding to (non-closed) classical solutions. We will study rather benign trajectories, however, it will already become evident what will happen for more generic and complicated solutions.

Using the potential  $V(\alpha, \phi) = e^{4\alpha} - m^2\phi^2e^{6\alpha}$  in (3.4), the constraint (4.13) translates to order  $\hbar$  into the following five quantum constraint functions

$$\begin{aligned}
C &= \langle \hat{p}_\phi \rangle^2 + (\Delta p_\phi)^2 - \langle \hat{p}_\alpha \rangle^2 - (\Delta p_\alpha)^2 - e^{4\langle \hat{\alpha} \rangle} - 8e^{4\langle \hat{\alpha} \rangle} (\Delta \alpha)^2 + m^2 \langle \phi \rangle^2 e^{6\langle \hat{\alpha} \rangle} \\
&\quad + m^2 e^{6\langle \hat{\alpha} \rangle} (\Delta \phi)^2 + 12m^2 \langle \phi \rangle e^{6\langle \hat{\alpha} \rangle} \Delta(\alpha \phi) + 18m^2 \langle \phi \rangle^2 e^{6\langle \hat{\alpha} \rangle} (\Delta \alpha)^2, \\
C_\alpha &= 2p_\phi \Delta(\alpha p_\phi) - 2p_\alpha \Delta(\alpha p_\alpha) - i\hbar p_\alpha + 2m^2 \phi e^{6\alpha} \Delta(\alpha \phi) + (6m^2 \phi^2 e^{6\alpha} - 4e^{4\alpha}) (\Delta \alpha)^2, \\
C_\phi &= 2p_\phi \Delta(\phi p_\phi) + i\hbar p_\phi - 2p_\alpha \Delta(\phi p_\alpha) + (6m^2 \phi^2 e^{6\alpha} - 4e^{4\alpha}) \Delta(\alpha \phi) + 2m^2 \phi e^{6\alpha} (\Delta \phi)^2, \\
C_{p_\alpha} &= 2p_\phi \Delta(p_\alpha p_\phi) - 2p_\alpha (\Delta p_\alpha)^2 + (6m^2 \phi^2 e^{6\alpha} - 4e^{4\alpha}) \Delta(\alpha p_\alpha) + 2m^2 \phi e^{6\alpha} \Delta(\phi p_\alpha) \\
&\quad - i\hbar (3m^2 \phi^2 e^{6\alpha} - 2e^{4\alpha}), \\
C_{p_\phi} &= 2p_\phi (\Delta p_\phi)^2 - 2p_\alpha \Delta(p_\alpha p_\phi) + (6m^2 \phi^2 e^{6\alpha} - 4e^{4\alpha}) \Delta(\alpha p_\phi) + 2m^2 \phi e^{6\alpha} \Delta(\phi p_\phi) \\
&\quad - i\hbar m^2 \phi e^{6\alpha}.
\end{aligned} \tag{4.17}$$

Due to the degeneracy in the quantum Poisson structure the five constraints (4.17) generate only four independent gauge flows. To remove redundant degrees of freedom, we choose a relational clock and a corresponding *Zeitgeist*, thereby fixing three of the four independent gauge flows. We are then left with just one (Hamiltonian) constraint governing the evolution of the system.

#### 4.3.1 Evolution in $\alpha$

Choosing  $\alpha$  as our relational clock, we resort to the  $\alpha$ -*Zeitgeist*

$$(\Delta \alpha)^2 = \Delta(\phi \alpha) = \Delta(\alpha p_\phi) = 0, \tag{4.18}$$

which, as can be easily checked by solving  $C_\alpha$ , leads to a saturation of the generalized uncertainty relation for the clock degrees of freedom. The rest of the constraints is simplified,

$$\begin{aligned}
C &= p_\phi^2 + (\Delta p_\phi)^2 - p_\alpha^2 - (\Delta p_\alpha)^2 - e^{4\alpha} + m^2 \phi^2 e^{6\alpha} + m^2 e^{6\alpha} (\Delta \phi)^2, \\
C_\phi &= 2p_\phi \Delta(\phi p_\phi) + i\hbar p_\phi - 2p_\alpha \Delta(\phi p_\alpha) + 2m^2 \phi e^{6\alpha} (\Delta \phi)^2, \\
C_{p_\alpha} &= 2p_\phi \Delta(p_\alpha p_\phi) - 2p_\alpha (\Delta p_\alpha)^2 + 2m^2 \phi e^{6\alpha} \Delta(\phi p_\alpha) - i\hbar(6m^2 \phi^2 e^{6\alpha} - 4e^{4\alpha}), \\
C_{p_\phi} &= 2p_\phi (\Delta p_\phi)^2 - 2p_\alpha \Delta(p_\alpha p_\phi) + 2m^2 \phi e^{6\alpha} \Delta(\phi p_\phi) - i\hbar m^2 \phi e^{6\alpha},
\end{aligned} \tag{4.19}$$

and can be used to solve for the unphysical moments  $\Delta(\phi p_\alpha), (\Delta p_\alpha)^2, \Delta(p_\alpha p_\phi)$ . Relational evolution of the remaining degrees of freedom in  $\alpha$  is generated by the remaining first-class (Hamiltonian) constraint which, by (3.6), in the  $\alpha$ -*Zeitgeist* reads

$$\begin{aligned}
C_H &= p_\phi^2 - p_\alpha^2 - e^{4\alpha} + m^2 \phi^2 e^{6\alpha} + \left[1 - \frac{p_\phi^2}{p_\alpha^2}\right] (\Delta p_\phi)^2 - \frac{2m^2 \phi e^{6\alpha} p_\phi}{p_\alpha^2} \Delta(\phi p_\phi) \\
&\quad + \left[m^2 e^{6\alpha} - \frac{m^4 \phi^2 e^{12\alpha}}{p_\alpha^2}\right] (\Delta \phi)^2 + i\hbar \frac{3m^2 \phi^2 e^{6\alpha} - 2e^{4\alpha}}{p_\alpha}.
\end{aligned} \tag{4.20}$$

Through the Poisson structure (2.2) this constraint generates the following equations of motion

$$\begin{aligned}
\dot{\alpha} &= -2p_\alpha + \frac{2p_\phi^2}{p_\alpha^3} (\Delta p_\phi)^2 + \frac{4m^2 \phi e^{6\alpha} p_\phi}{p_\alpha^3} \Delta(\phi p_\phi) + \frac{2m^4 \phi^2 e^{12\alpha}}{p_\alpha^3} (\Delta \phi)^2 - i\hbar \frac{3m^2 \phi^2 e^{6\alpha} - 2e^{4\alpha}}{p_\alpha^2}, \\
\dot{p}_\alpha &= 4e^{4\alpha} - 6m^2 \phi^2 e^{6\alpha} + \frac{12m^2 \phi e^{6\alpha} p_\phi}{p_\alpha^2} \Delta(\phi p_\phi) - \left[6m^2 e^{6\alpha} - \frac{12m^4 \phi^2 e^{12\alpha}}{p_\alpha^2}\right] (\Delta \phi)^2 \\
&\quad - i\hbar \frac{18m^2 \phi^2 e^{6\alpha} - 8e^{4\alpha}}{p_\alpha}, \\
\dot{\phi} &= 2p_\phi - \frac{2p_\phi}{p_\alpha^2} (\Delta p_\phi)^2 - \frac{2m^2 \phi e^{6\alpha}}{p_\alpha^2} \Delta(\phi p_\phi), \\
\dot{p}_\phi &= -2m^2 \phi e^{6\alpha} + \frac{2m^2 e^{6\alpha} p_\phi}{p_\alpha^2} \Delta(\phi p_\phi) + \frac{2m^4 \phi e^{12\alpha}}{p_\alpha^2} (\Delta \phi)^2 - i\hbar \frac{6m^2 \phi e^{6\alpha}}{p_\alpha}, \\
(\Delta \dot{\phi})^2 &= 4 \left[1 - \frac{p_\phi^2}{p_\alpha^2}\right] \Delta(\phi p_\phi) - \frac{4m^2 \phi e^{6\alpha} p_\phi}{p_\alpha^2} (\Delta \phi)^2, \\
\Delta(\dot{\phi} p_\phi) &= 2 \left[1 - \frac{p_\phi^2}{p_\alpha^2}\right] (\Delta p_\phi)^2 + 2 \left[\frac{m^4 \phi^2 e^{12\alpha}}{p_\alpha^2} - m^2 e^{6\alpha}\right] (\Delta \phi)^2, \\
(\Delta \dot{p}_\phi)^2 &= \frac{4m^2 \phi e^{6\alpha} p_\phi}{p_\alpha^2} (\Delta p_\phi)^2 + 4 \left[-m^2 e^{6\alpha} + \frac{m^4 \phi^2 e^{12\alpha}}{p_\alpha^2}\right] \Delta(\phi p_\phi).
\end{aligned} \tag{4.21}$$

As in [3, 4], it is straightforward to show that the evolving degrees of freedom in the  $\alpha$ -*Zeitgeist*, i.e.  $\phi, p_\phi, (\Delta \phi)^2, (\Delta \phi p_\phi)$  and  $(\Delta p_\phi)^2$ , can be consistently chosen real if  $\alpha$  picks up the imaginary part (3.8) (with  $q_1, p_1$  replaced by  $\alpha, p_\alpha$ ). The set (4.21) can be solved numerically,

yielding the evolution of the transient observables of the  $\alpha$ -*Zeitgeist* (i.e. the correlations of the evolving variables with  $\Re[\alpha]$ ).

As generally discussed in section 3.1, the  $\alpha$ -*Zeitgeist* possesses only a transient validity because  $\alpha$  is a non-global clock. To remedy this issue in the turning region(s) of  $\alpha$ , we will choose  $\phi$  as the new clock and evolve the system in the  $\phi$ -*Zeitgeist* instead.

### 4.3.2 Evolution in $\phi$

The  $\phi$ -*Zeitgeist*,

$$(\Delta\phi)^2 = \Delta(\alpha\phi) = \Delta(\phi p_\alpha) = 0, \quad (4.22)$$

by solving  $C_\phi$ , leads to a saturation of the generalized uncertainty relation for the pair  $(\phi, p_\phi)$ . The rest of the constraints is now given by

$$\begin{aligned} C &= p_\phi^2 + (\Delta p_\phi)^2 - p_\alpha^2 - (\Delta p_\alpha)^2 - e^{4\alpha} + m^2 \phi^2 e^{6\alpha} + (18m^2 \phi^2 e^{6\alpha} - 8e^{4\alpha})(\Delta\alpha)^2, \\ C_\alpha &= 2p_\phi \Delta(\alpha p_\phi) - 2p_\alpha \Delta(\alpha p_\alpha) - i\hbar p_\alpha + (6m^2 \phi^2 e^{6\alpha} - 4e^{4\alpha})(\Delta\alpha)^2, \\ C_{p_\alpha} &= 2p_\phi \Delta(p_\alpha p_\phi) - 2p_\alpha (\Delta p_\alpha)^2 + (6m^2 \phi^2 e^{6\alpha} - 4e^{4\alpha})\Delta(\alpha p_\alpha) - i\hbar (3m^2 \phi^2 e^{6\alpha} - 2e^{4\alpha}), \\ C_{p_\phi} &= 2p_\phi (\Delta p_\phi)^2 - 2p_\alpha \Delta(p_\alpha p_\phi) + (6m^2 \phi^2 e^{6\alpha} - 4e^{4\alpha})\Delta(\alpha p_\phi) - 2i\hbar m^2 \phi e^{6\alpha}, \end{aligned} \quad (4.23)$$

and, again, can be used to solve for the unphysical moments  $\Delta(\alpha p_\phi)$ ,  $\Delta(p_\alpha p_\phi)$ ,  $(\Delta p_\phi)^2$ .

The Hamiltonian constraint in  $\phi$ -*Zeitgeist* reads

$$\begin{aligned} C_H &= p_\phi^2 - p_\alpha^2 - e^{4\alpha} + m^2 \phi^2 e^{6\alpha} - \left[ 1 - \frac{p_\alpha^2}{p_\phi^2} \right] (\Delta p_\alpha)^2 - \frac{p_\alpha}{p_\phi^2} (6m^2 \phi^2 e^{6\alpha} - 4e^{4\alpha}) \Delta(\alpha p_\alpha) \\ &\quad + \left[ 18m^2 \phi^2 e^{6\alpha} - 8e^{4\alpha} + \frac{(3m^2 \phi^2 e^{6\alpha} - 2e^{4\alpha})^2}{p_\phi^2} \right] (\Delta\alpha)^2 + i\hbar \frac{m^2 \phi e^{6\alpha}}{p_\phi} \end{aligned} \quad (4.24)$$

and generates the following set of equations of motion for  $\alpha$ ,  $p_\alpha$ ,  $(\Delta\alpha)^2$ ,  $(\Delta p_\alpha)^2$  and  $\Delta(\alpha p_\alpha)$  which constitute the evolving degrees of freedom in the  $\phi$ -*Zeitgeist*

$$\begin{aligned} \dot{\phi} &= 2p_\phi - \frac{2p_\alpha^2}{p_\phi^3} (\Delta p_\alpha)^2 + \frac{p_\alpha}{p_\phi^3} (12m^2 \phi^2 e^{6\alpha} - 8e^{4\alpha}) \Delta(\alpha p_\alpha) - \frac{(6m^2 \phi^2 e^{6\alpha} - 4e^{4\alpha})^2}{2p_\phi^3} (\Delta\alpha)^2 \\ &\quad - i\hbar \frac{m^2 \phi e^{6\alpha}}{p_\phi^2}, \\ \dot{p}_\phi &= -2m^2 \phi e^{6\alpha} + \frac{12p_\alpha}{p_\phi^2} m^2 \phi e^{6\alpha} \Delta(\alpha p_\alpha) - \left[ 36m^2 \phi e^{6\alpha} + \frac{12m^2 \phi e^{6\alpha} (3m^2 \phi^2 e^{6\alpha} - 2e^{4\alpha})}{p_\phi^2} \right] (\Delta\alpha)^2 \\ &\quad - i\hbar \frac{m^2 e^{6\alpha}}{p_\phi}, \\ \dot{\alpha} &= -2p_\alpha + \frac{2p_\alpha}{p_\phi^2} (\Delta p_\alpha)^2 - \frac{6m^2 \phi^2 e^{6\alpha} - 4e^{4\alpha}}{p_\phi^2} \Delta(\alpha p_\alpha), \end{aligned} \quad (4.25)$$

$$\begin{aligned}
\dot{p}_\alpha &= 4e^{4\alpha} - 6m^2\phi^2e^{6\alpha} + \frac{p_\alpha}{p_\phi^2}(36m^2\phi^2e^{6\alpha} - 16e^{4\alpha})\Delta(\alpha p_\alpha) - i\hbar \frac{6m^2\phi e^{6\alpha}}{p_\phi} \\
&\quad - \left[ 108m^2\phi^2e^{6\alpha} - 32e^{4\alpha} + \frac{(18m^2\phi^2e^{6\alpha} - 8e^{4\alpha})(6m^2\phi^2e^{6\alpha} - 4e^{4\alpha})}{p_\phi^2} \right] (\Delta\alpha)^2, \\
(\dot{\Delta\alpha})^2 &= -4 \left[ 1 - \frac{p_\alpha^2}{p_\phi^2} \right] \Delta(\alpha p_\alpha) - \frac{p_\alpha}{p_\phi^2}(12m^2\phi^2e^{6\alpha} - 8e^{4\alpha})(\Delta\alpha)^2, \\
\Delta(\dot{\alpha p_\alpha}) &= -2 \left[ 1 - \frac{p_\alpha^2}{p_\phi^2} \right] (\Delta p_\alpha)^2 - 2 \left[ 18m^2\phi^2e^{6\alpha} - 8e^{4\alpha} + \frac{(3m^2\phi^2e^{6\alpha} - 2e^{4\alpha})^2}{p_\phi^2} \right] (\Delta\alpha)^2, \\
(\Delta\dot{p}_\alpha)^2 &= \frac{p_\alpha}{p_\phi^2}(12m^2\phi^2e^{6\alpha} - 8e^{4\alpha})(\Delta p_\alpha)^2 - 4 \left[ 18m^2\phi^2e^{6\alpha} - 8e^{4\alpha} + \frac{(3m^2\phi^2e^{6\alpha} - 2e^{4\alpha})^2}{p_\phi^2} \right] \Delta(\alpha p_\alpha).
\end{aligned}$$

Once more, the clock variable  $\phi$  develops a complex nature, in agreement with (3.8),  $\text{Im } \phi = -\frac{\hbar}{2p_\phi}$ , while the evolving degrees of freedom can be chosen real.

### 4.3.3 Numerical results

We now analyze the numerical behavior of the truncated effective system that starts off peaked about classical trajectories for which neither the scalar field nor the scale factor are good global clocks. For simplicity, we restrict our attention to a special class of trajectories—those that have very few local extrema in the scale factor: in a more general case the internal clocks would need to be switched many times in order to evolve through the bouncing part of the trajectory. The cases considered are sufficient to illustrate several qualitative points that apply more generally, in particular, that changing the clock in the region of maximal expansion will not work in a generic solution.

Figure 4(a) displays an effective relational trajectory in the configuration space that was patched together by first evolving it using  $\alpha$  as a clock, followed by transforming to the  $\phi$ -*Zeitgeist* between the extremal points  $\phi = \phi_{\min}$  and  $\alpha = \alpha_{\max}$ , finally switching back to the  $\alpha$ -*Zeitgeist* after  $\alpha = \alpha_{\max}$ , but before  $\phi = \phi_{\max}$ . Alongside the effective trajectory, figure 4(a) displays the corresponding classical trajectory, with the two being virtually indistinguishable. For the particular numerical evolution plotted we chose the quantum scale such that  $\sqrt{\hbar} \sim 10^{-4}$  when compared to the expectation values that are of order 1. The leading order quantum corrections are of order  $\hbar$  and are therefore  $\sim 10^{-8}$  times weaker than the classical effects. In this regime the quantum back-reaction is virtually non-existent and the classical variables evolve essentially independently from the quantum modes. The necessity for this large separation of the classical and quantum scales chosen ultimately traces back to the classical chaoticity of the system and can be illustrated by the behavior of the moments in figures 4(b)–5(b). The initial values of the moments in the  $\alpha$ -*Zeitgeist* are close to  $\hbar$ , however, at a certain point in the outgoing trajectory they are about  $10^4$  times larger than their initial values, which makes the assumption about the semiclassical fall-off outright inapplicable if the separation of the different perturbative orders is less than  $10^4$ . The defocussing of classical trajectories in the region of maximal expansion forces a semiclassical state initially peaked on nearby classical trajectories to inevitably spread apart yielding an overall growth of the moments. For the classical solution reproduced by the effective solution in figure 4(a), the defocussing of initially neighboring trajectories is displayed in figure 3. Furthermore, the “spikes” in the moments,

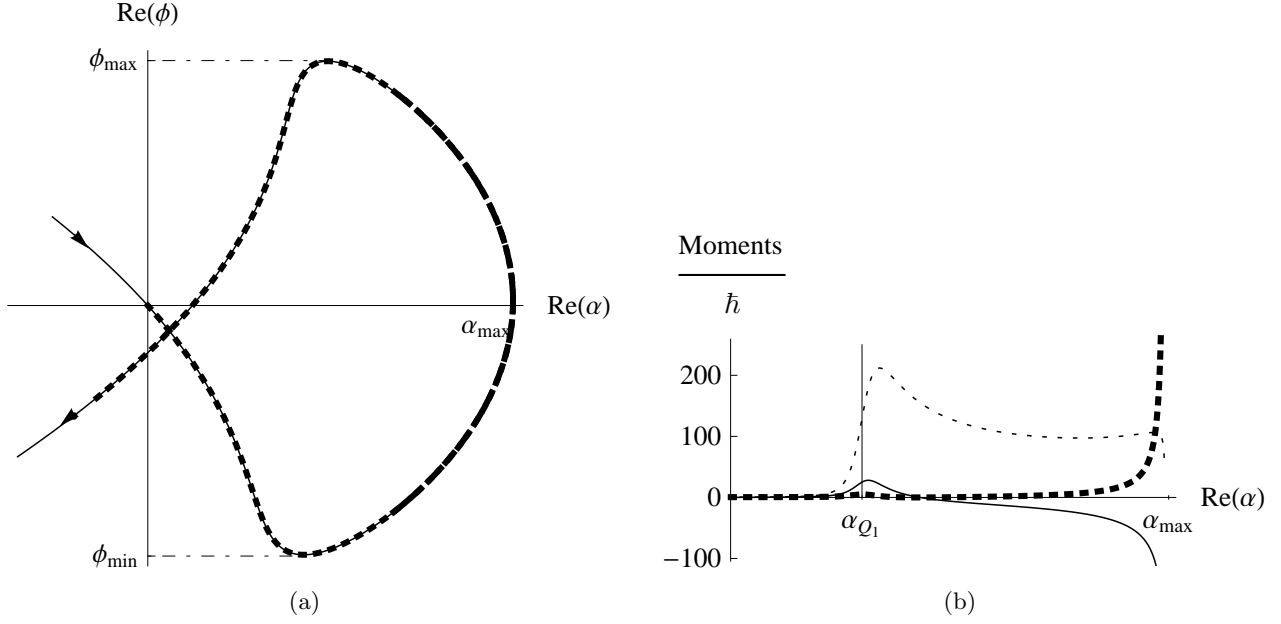


Figure 4: (a) Classical trajectory (dotted) and patched up effective trajectory:  $\alpha$ -gauge (solid),  $\phi$ -gauge (dashed). (b) Moments in  $\alpha$ -gauge on the incoming branch:  $(\Delta\phi)^2$  (thick, dashed),  $(\Delta p_\phi)^2$  (thin, dashed),  $\Delta(\phi p_\phi)$  (solid).  $\alpha_{Q_1}$  is the quasi-turning point of  $\alpha$  on the incoming branch where the clock becomes ‘slow’ (see discussion and figure 6(a)).

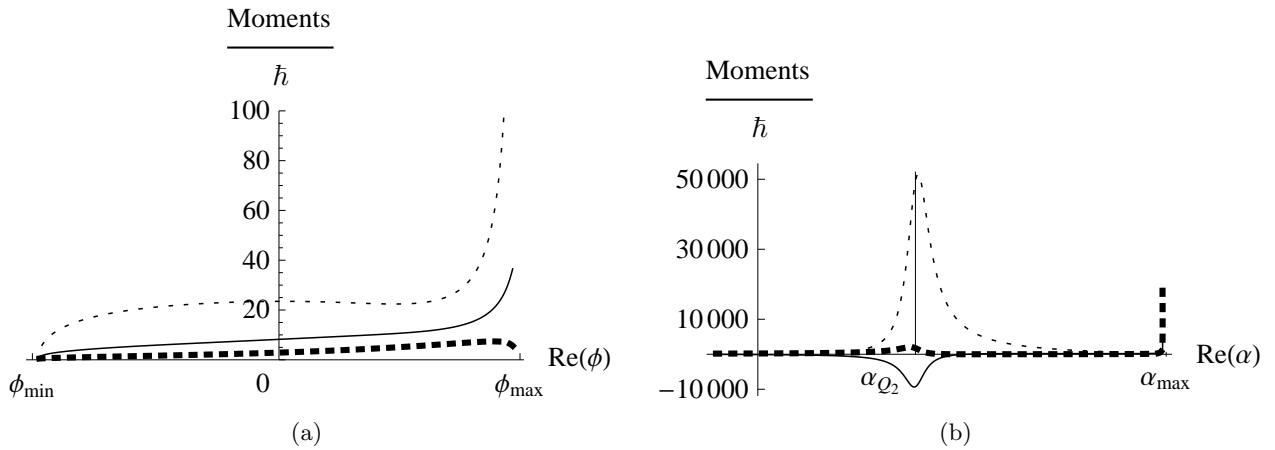


Figure 5: (a) Moments in  $\phi$ -gauge:  $(\Delta\alpha)^2$  (thick, dashed),  $(\Delta p_\alpha)^2$  (thin, dashed),  $\Delta(\alpha p_\alpha)$  (solid). (b) Moments in  $\alpha$ -gauge on the outgoing branch:  $(\Delta\phi)^2$  (thick, dashed),  $(\Delta p_\phi)^2$  (thin, dashed),  $\Delta(\phi p_\phi)$  (solid).  $\alpha_{Q_2}$  is the quasi-turning point of  $\alpha$  on the outgoing branch where the clock becomes ‘slow’ (see discussion and figure 6(b)).



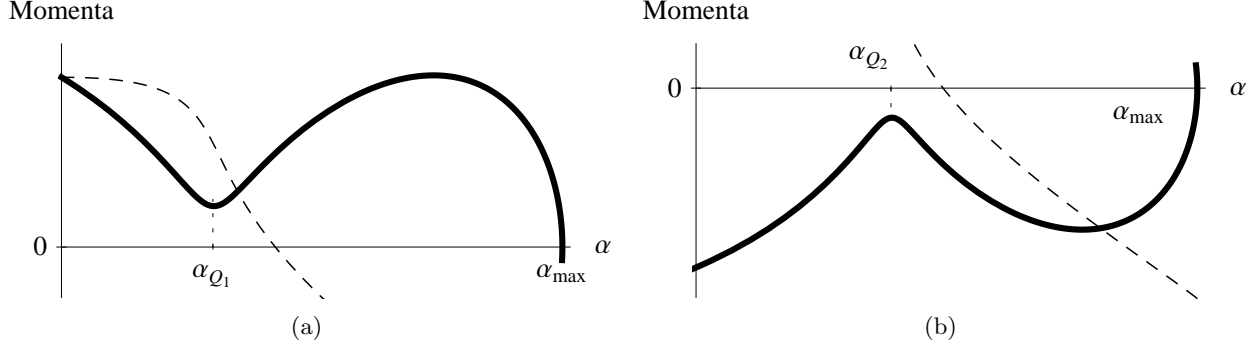


Figure 6: (a) Classical momenta on the incoming branch with quasi-turning point  $\alpha_{Q_1}$  of the clock  $\alpha$ :  $p_\phi$  (dashed),  $p_\alpha$  (solid). (b) Classical momenta on the outgoing branch with quasi-turning point  $\alpha_{Q_2}$ :  $p_\phi$  (dashed),  $p_\alpha$  (solid).

particularly  $(\Delta p_\phi)^2$ , in figures 4(b) and 5(b) trace their origin to the classical quasi-turning points of the internal clock  $\alpha = \alpha_{Q_1}$  and  $\alpha = \alpha_{Q_2}$ , where  $\dot{\alpha} = -2p_\alpha$  is small and the clock  $\alpha$  thus becomes ‘too slow’ for resolving the evolution of other degrees of freedom with respect to it (also see discussion in section 3.1). One might suggest evolving through these regions using  $\phi$  as the internal clock, however this may not be feasible as the quasi-turning points in  $\alpha$  may lie too close to the turning points in  $\phi$ : for the particular trajectory this is illustrated in figures 6(a) and 6(b) for the incoming and outgoing branches respectively, where one can see the proximity of the local minima in  $p_\alpha$  and the points where  $p_\phi = 0$ . Both  $\alpha$  and  $\phi$  (as well as their momenta) are thus ‘bad clocks’ in immediate vicinity, leading to a poor resolution of relational evolution and thus to a large growth of the moments; no clock change can cure this ailment. As can be inferred from the general characterization of classical solutions given in [26], this property is a generic one in the space of solutions and thus will generically impede a good resolution of transient quantum observables.

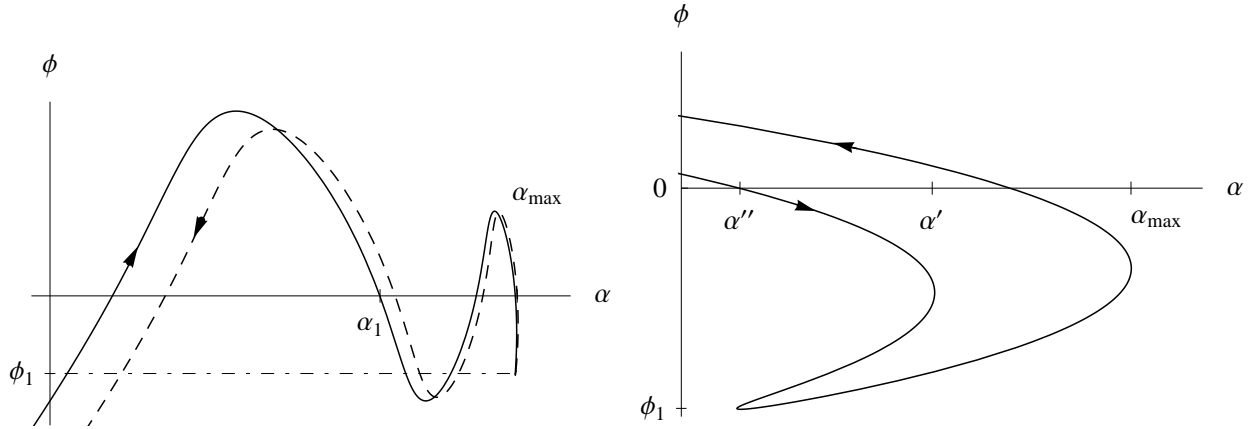


Figure 7: Left: a classical configuration-space trajectory computed using the same model parameters as in figure 4(a), but with different initial conditions: incoming branch (solid), outgoing branch (dashed). Right: a closeup of the same trajectory near  $\alpha = \alpha_{max}$ ; there are two other local extrema in  $\alpha$  labeled by  $\alpha'$  (a maximum) and  $\alpha''$  (a minimum), in addition, there  $\phi$  reaches a locally minimal value  $\phi_1$  very near  $\alpha = \alpha''$ .

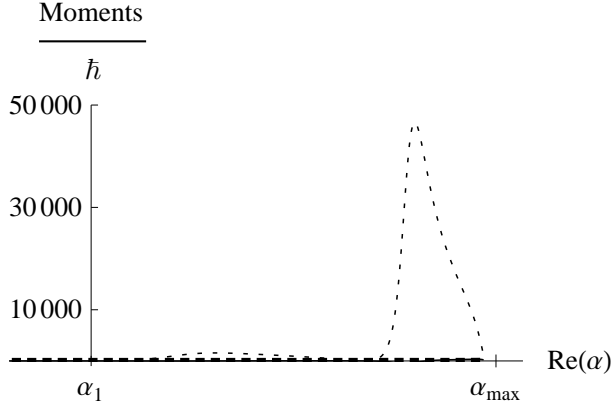


Figure 8: Moments in  $\alpha$ -gauge on the incoming branch evolved effectively in a state initially peaked around the trajectory in figure 7 :  $(\Delta\phi)^2$  (thick, dashed),  $(\Delta p_\phi)^2$  (thin, dashed),  $\Delta(\phi p_\phi)$  (solid).

The above problem is a manifestation of a more general issue in this model: an arbitrary classical trajectory can exhibit structure, such as local maxima and minima, at all scales—there is no natural threshold scale below which there is no classical structure. We illustrate this further by picking a slightly more complicated classical trajectory, plotted in figure 7. This trajectory uses the same model parameters (namely  $m$  and  $\hbar$ ) as the one in figure 4(a), with different initial conditions. The scale factor exhibits not one, but three local extrema at  $\alpha = \alpha_{max}, \alpha', \alpha''$ . The corresponding effective system is much more unstable already along the incoming branch when evolved in  $\alpha$ , so much so that by the time it approaches the classical turning points in  $\alpha$ , the spreads are of order comparable to the separation between the three extrema of  $\alpha$  (figure 8). The situation is, in fact, even worse, as the separation between the turning point of  $\phi$ , where  $\phi = \phi_1$ , and the local minimum in  $\alpha$ , where  $\alpha = \alpha''$ , is of order  $\sqrt{\hbar}$ , and the two points could not be resolved even if the moments remained well-behaved. Therefore, given the chosen quantum scale, this fairly benign trajectory cannot be resolved by the effective evolution as it stands. This result generalizes: for any given choice of the quantum scale there will be an infinite set of classical trajectories with extrema in  $\alpha$  and  $\phi$  separated on or below that scale [26], for such trajectories it is then fundamentally impossible, using the effective method, to construct entire semiclassical states which evolve nicely through the region of maximal expansion.

## 5 Conclusions

The present work is a first step in the study of relational quantum dynamics in the generic non-integrable case featuring a non-trivial coupling between the clock and the evolving degrees of freedom. The effective approach [3, 4] seems especially well-gearred for investigating semiclassical relational dynamics of non-integrable systems because it enables one to make sense of temporally local time evolution, yielding transient relational observables and allowing one to switch back and forth between various clock variables.

In particular, we have applied the effective approach to the (non-integrable) closed FRW model universe filled with a minimally coupled massive scalar field whose quantum dynamics have thus far not been properly studied. The numerical results obtained here for rather benign trajectories already demonstrate that semiclassicality in this cosmological model is a delicate issue in the region of maximal expansion and generally fails due to the sensitivity of solutions to the initial conditions which results in a generic defocussing of classical trajectories in this region; a semiclassical state peaked on initially nearby classical trajectories inevitably has to spread apart. This distinguishes the present cosmological model from the toy models earlier

studied in [4] where coherent states are available which are sharply peaked even in the turning region of the non-global clocks which, furthermore, are decoupled such that the imperfectness of one clock does not depend on that of the other.

The region of maximal expansion, in fact, features a chaotic scattering [28] which renders it especially challenging for relational dynamics. Indeed, the effective results reported here provide evidence that relational dynamics, while possible for sufficiently sharply peaked states, generically breaks down in the region of maximal expansion. In this regime, we can no longer trust the effective semiclassical truncation since the moments grow beyond order  $\sqrt{\hbar}$  and eventually diverge despite quantum back-reaction not playing a prominent role; no change of clock and *Zeitgeist* can remedy this. In particular, a generic classical trajectory exhibits quasi-turning points of the clock  $\alpha$  immediately following/preceding a turning point of the field  $\phi$  [26]; the two clock momenta thus become small (or vanish) in immediate neighborhood, rendering both clocks ‘too slow’ in order to properly resolve relational evolution [3, 4, 7, 8, 9, 46] and yielding large uncertainties. (In addition, the momenta of the two clocks do not fare any better as clocks themselves because they are generically highly oscillatory in nature.) It is evident, that in a situation more generic and featuring arbitrarily many more oscillations in both  $\alpha$  and  $\phi$  than the benign trajectories studied here, the situation will only get worse. However, as argued in [3], the failure of the effective semiclassical truncation in this manner, nevertheless, is strong evidence, suggesting that relational evolution generally breaks down due to a mixing of internal time directions in such a regime. This is the effective analogue of non-unitarity in a (local) deparametrization at a Hilbert space level resulting in a breakdown of (any) inner product based on level surfaces of the non-global clock variable.

The generic breakdown of semiclassicality in the region of maximal expansion is compatible with the necessary breakdown of the WKB approximation to (4.13) earlier reported in the literature [23, 24, 28, 29, 30]. Note, however, that while the WKB approximation is a specific method to study the semiclassical limit, here we have employed a very general semiclassical approximation. Indeed, in contrast to the arguments put forward in [5, 24, 30] concerning the semiclassical limit as obtained by WKB techniques, in the effective approach it *is* possible to obtain semiclassical solutions which follow a classical trajectory *without* continuous measurement through higher degrees of freedom if the state is initially sufficiently sharply peaked and the corresponding classical trajectory sufficiently benign. One merely has to switch the relational clock at intermediate stages according to the general construction presented in this article. For these sufficiently peaked states the (relational) IVP retrieves its classical (deterministic) character of having the re-collapsing branch as the logical successor of the expanding one—this, once more, stands in contrast to the discussion in [5, 24, 30]. Although, clearly, the recovery of a ‘good (temporally) local relational evolution’ depends very sensitively on the state.

As a consequence of non-integrability being the generic case in dynamical systems [14], we conjecture that the reported qualitative results concerning (the breakdown of) relational evolution and semiclassicality (ultimately rooted in the non-integrability) should feature prominently in a generic situation in quantum cosmology and gravity, thus emphasizing the delicate nature of the question posed in the beginning. Generically, ‘good relational evolution’ appears to be only a transient and semiclassical phenomenon.

However, non-integrability manifests itself in sensitivity to initial data. A natural question to ask is whether loop quantum cosmology, which possesses a minimal length scale originating in the minimal area gap [11, 12] (giving ‘infinitesimally close’ a different notion), could possibly resolve any chaotic attributes of this model universe, thereby providing a ‘better behaved’ theory.

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